

CRITICAL ISSUES WITH QUANTIFICATION OF DISCRETIZATION UNCERTAINTY IN CFD

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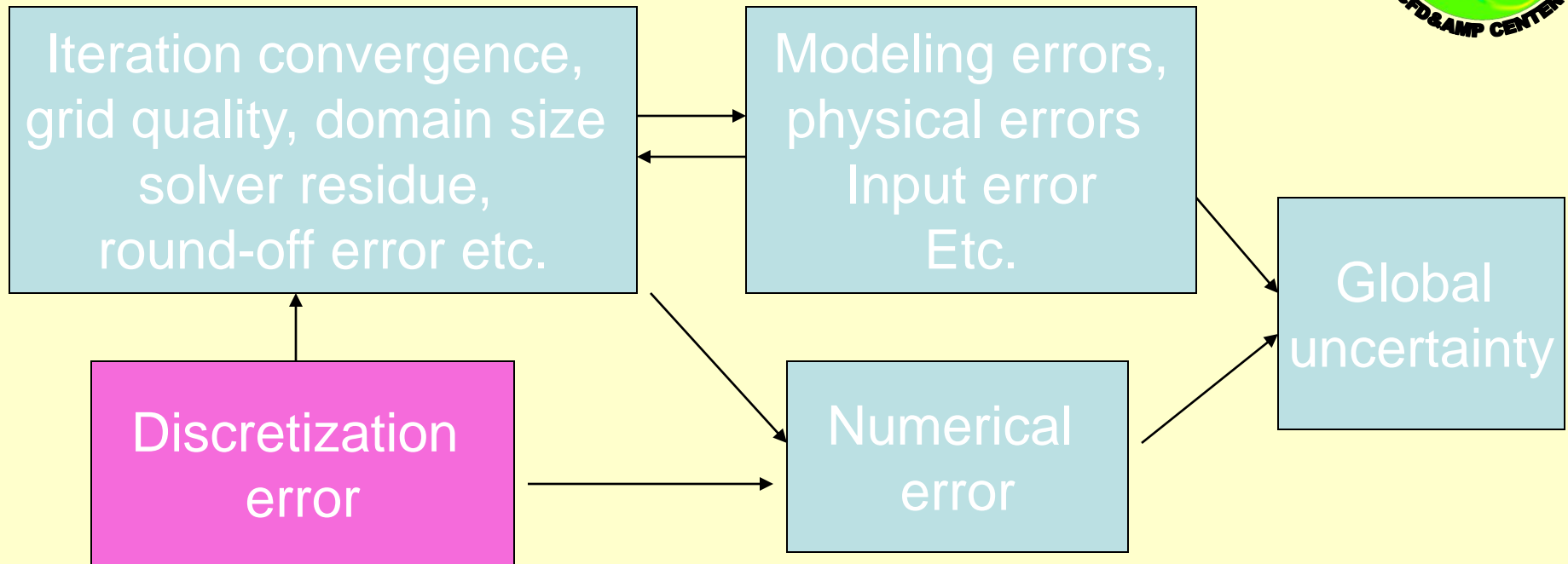
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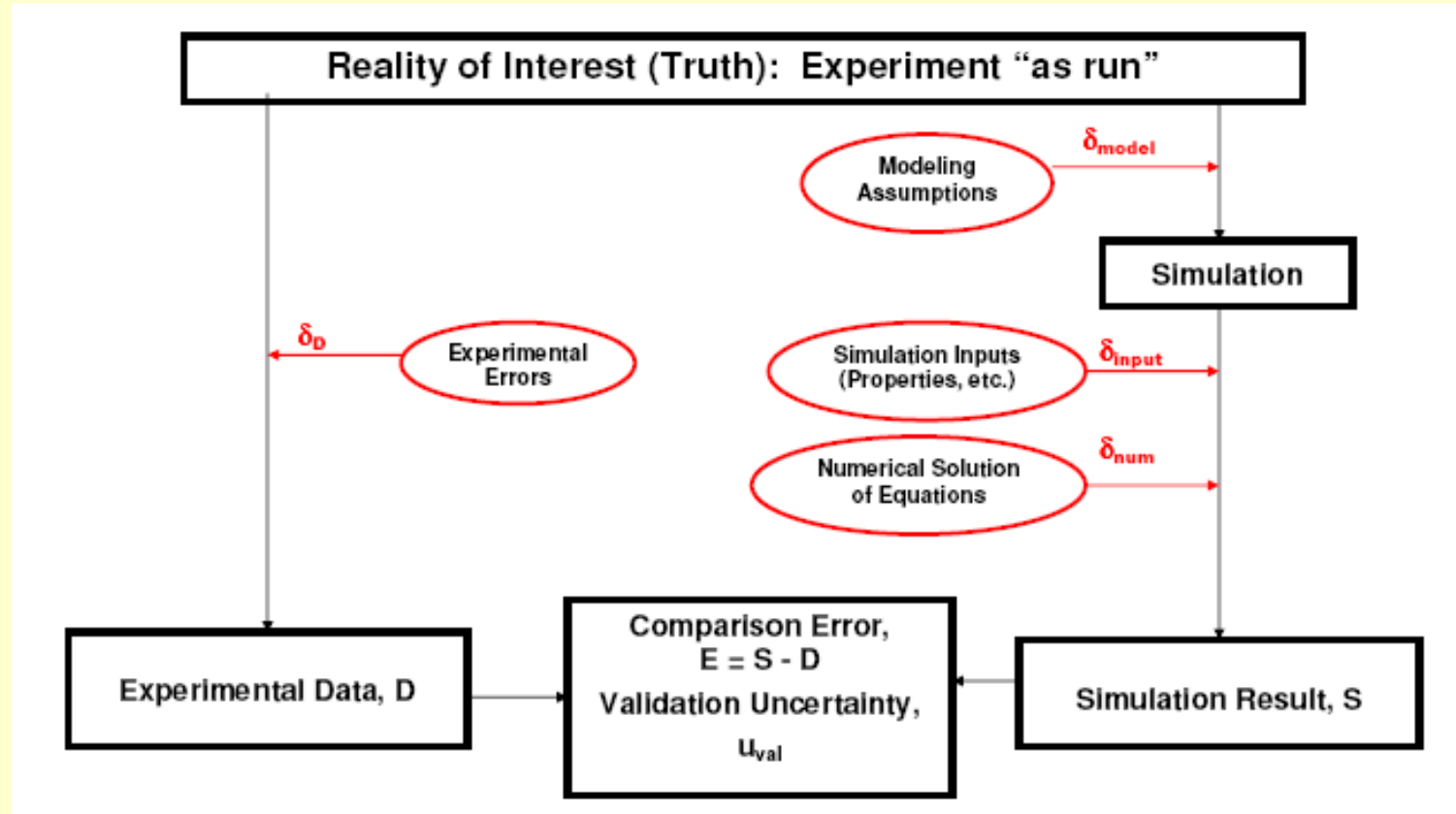
Errors and Uncertainty!



Common methods of quantifying discretization error:

- **Zhu-Zienkiewicz (ZZ) and energy norm methods**
 - Richardson extrapolation (RE)
 - Error transport method (ETE)
- Hybrid ETE and Residual Methods

V&V Overview*



$$E = \delta_{\text{model}} + \delta_{\text{input}} + \delta_{\text{num}} - \delta_D \quad u_{\text{val}} = \sqrt{u_D^2 + u_{\text{num}}^2 + u_{\text{input}}^2}^{\frac{1}{2}}$$

* After Coleman (see e.g. ASME V&V 20, 2010)

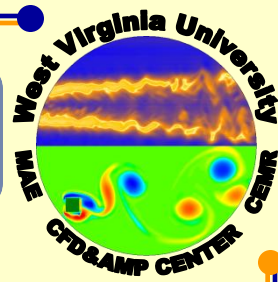
On the question of determinism

- “ ... the randomness of quantum mechanics is like a coin toss*. It looks random, but it's not really random.”

Carsten van de Bruck

- from Musser , G. (2004) ‘Was Einstein Right?’ Scientific American September issue, pp. 88-91
- * *All coins tossed from a skyscraper with different initial velocities will reach the same terminal velocity due to friction loss (i.e. information loss)*

Error Analysis: Deterministic Methods



Goal: Assessment of all types of numerical errors and modeling errors with repeatable (deterministic) calculations.

Calculation Verification: A calculation is what it is supposed to be in the context of numerical analysis, i.e. the equations (PDE's) are solved right!
(After P. Roache)

In practice: Assess grid convergence

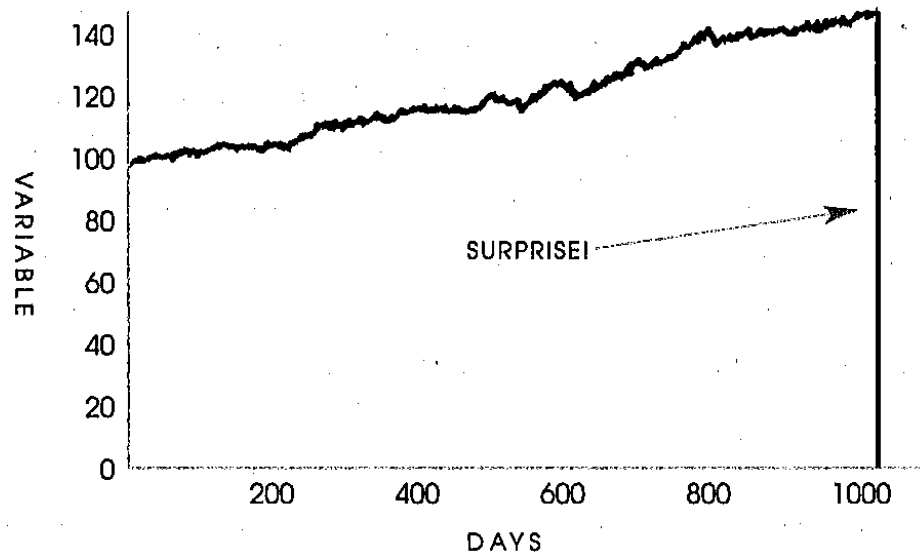
Validation: Assessment of modeling errors in conjunction with verification:
Compare with Experiments, DNS, Observations, Perceptions

- ***Paradox: Determinism \leftrightarrow Randomness/surprise/unpredictable***

The Black Swan Phenomenon:

White swans, gray swans, and black swans

FIGURE 1: ONE THOUSAND AND ONE DAYS OF HISTORY



A turkey before and after Thanksgiving. The history of a process over a thousand days tells you nothing about what is to happen next. This naïve projection of the future from the past can be applied to anything.

Ref.: *The Black Swan, The impact of the highly improbable* by N.N. Taleb, 2010, Random House

Numerical Dissipation is Always There!

- Theoretical analysis by Ghosal (1996, *J. Comp. Phys*, 125, pp. 187-206) concludes:
 - **Finite Diff. Error** = **const** * λ^q ; λ is the wave number, $q = \text{const} = 0.75$ and independent of the scheme, *const* varies with the scheme (1.03 for 2nd order CD, 0.5 for 8th order CD)
- Choi and Moin (1994): 2nd order methods have certain advantages, and ‘higher order’ is not necessarily better.
- Even with higher order methods Numerical dissipation can be as large as the modeling error, and may cancel each better.

The key question: *How do the numerical errors interact with modeling errors?*

Uncertainty of Numerical Solutions

Implicit Solution

Explicit Solution

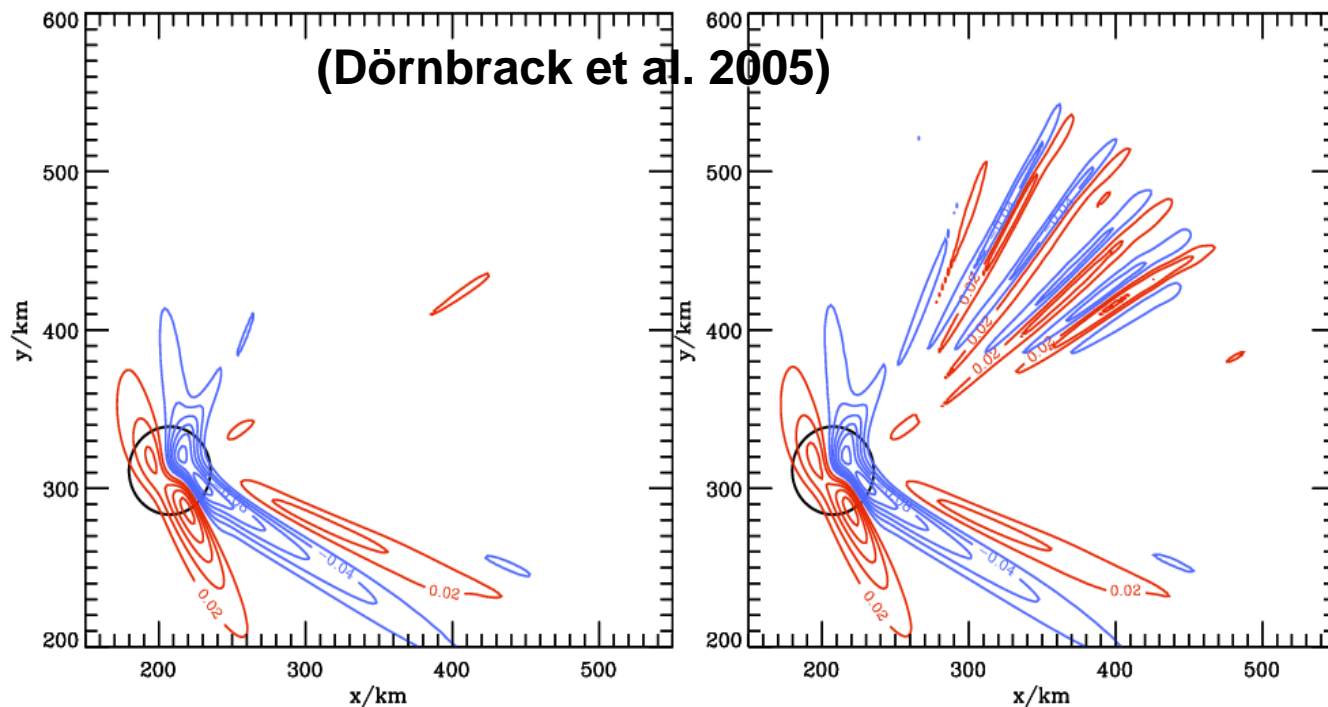
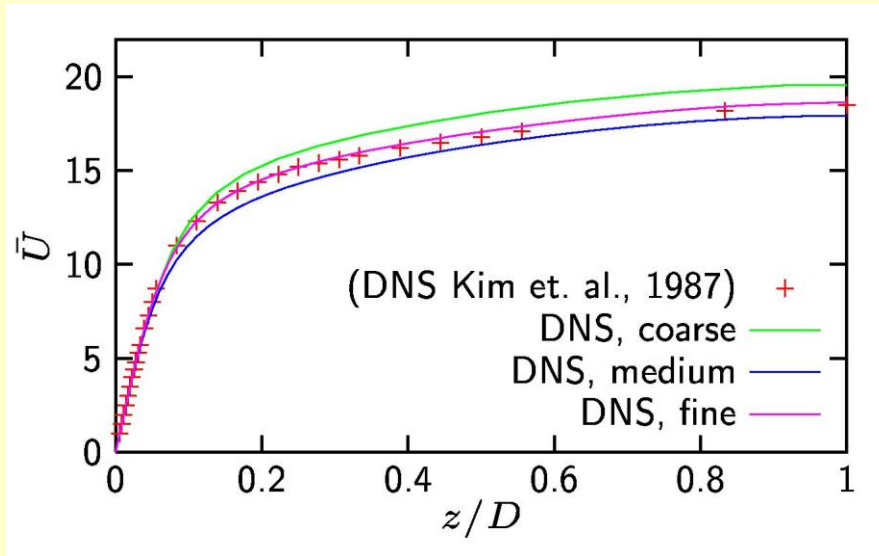
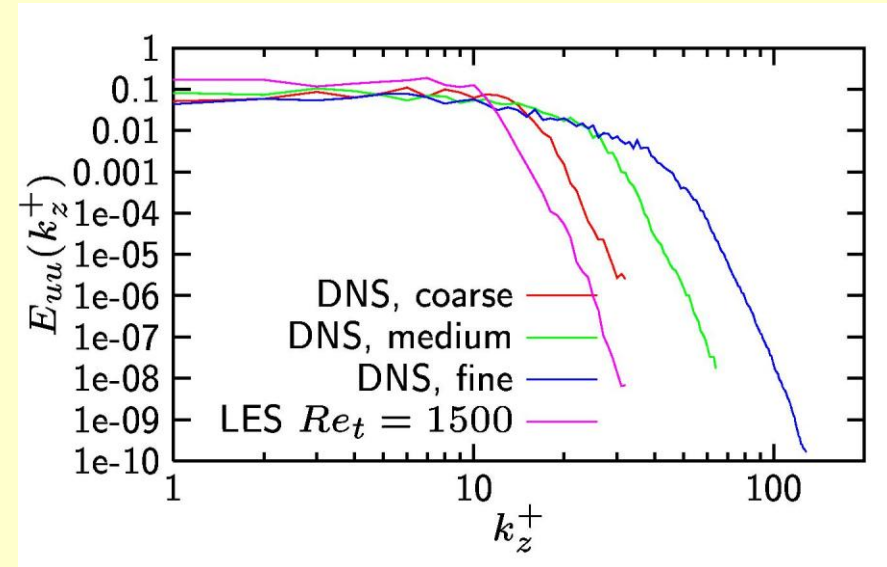


Figure 1: Vertical velocity with contour interval $\Delta w = 0.02$ m/s (red positive, blue negative) at $z = 6$ km altitude, after 6 h integration time for the implicit (left) and explicit simulation (right). The black line marks the 100 m elevation contour line.

Numerical dissipation & Effective Re



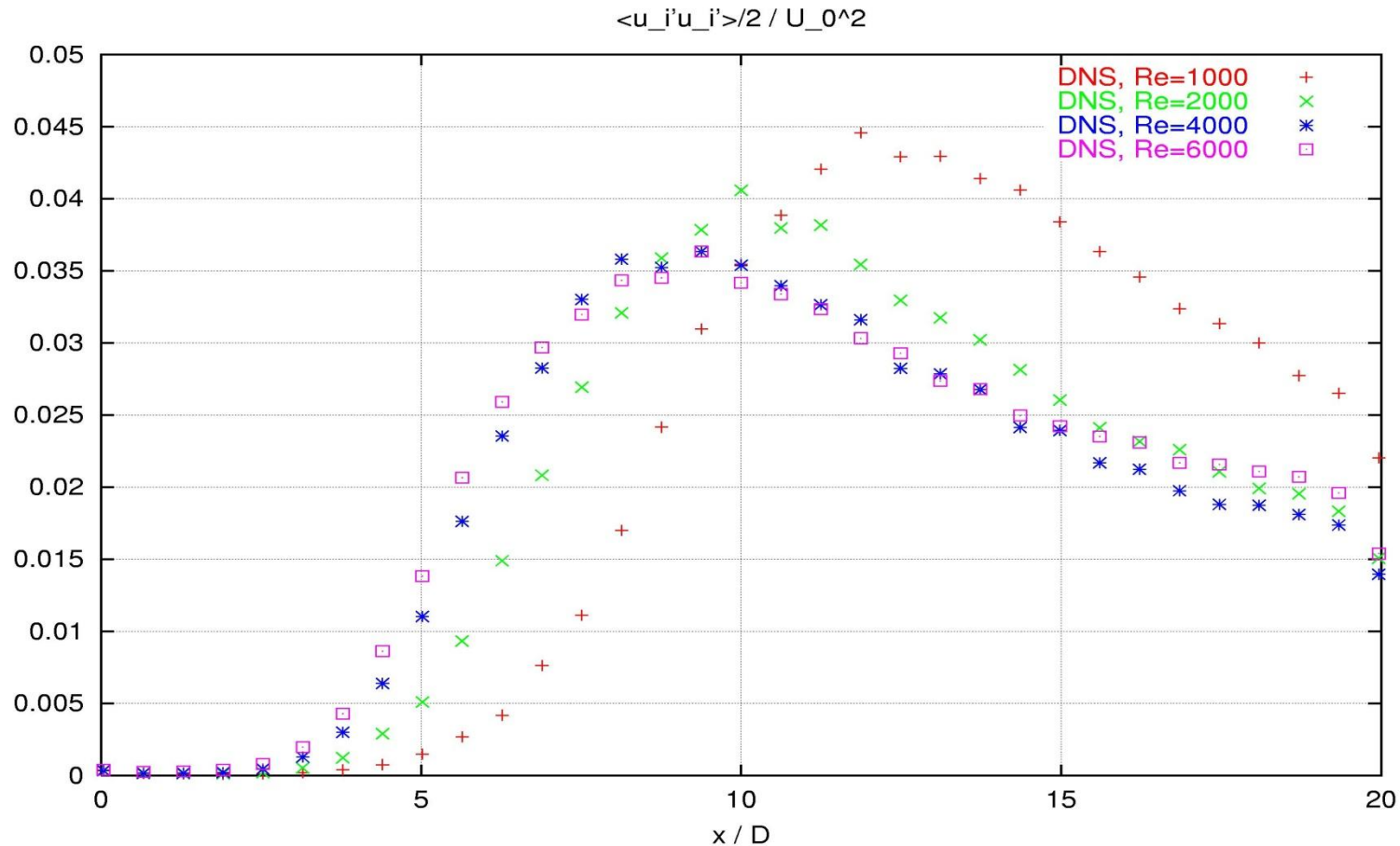
Mean velocity profile



Energy spectra

Data: Courtesy of Dr. Ing. Markus Klein (2005); Channel flow

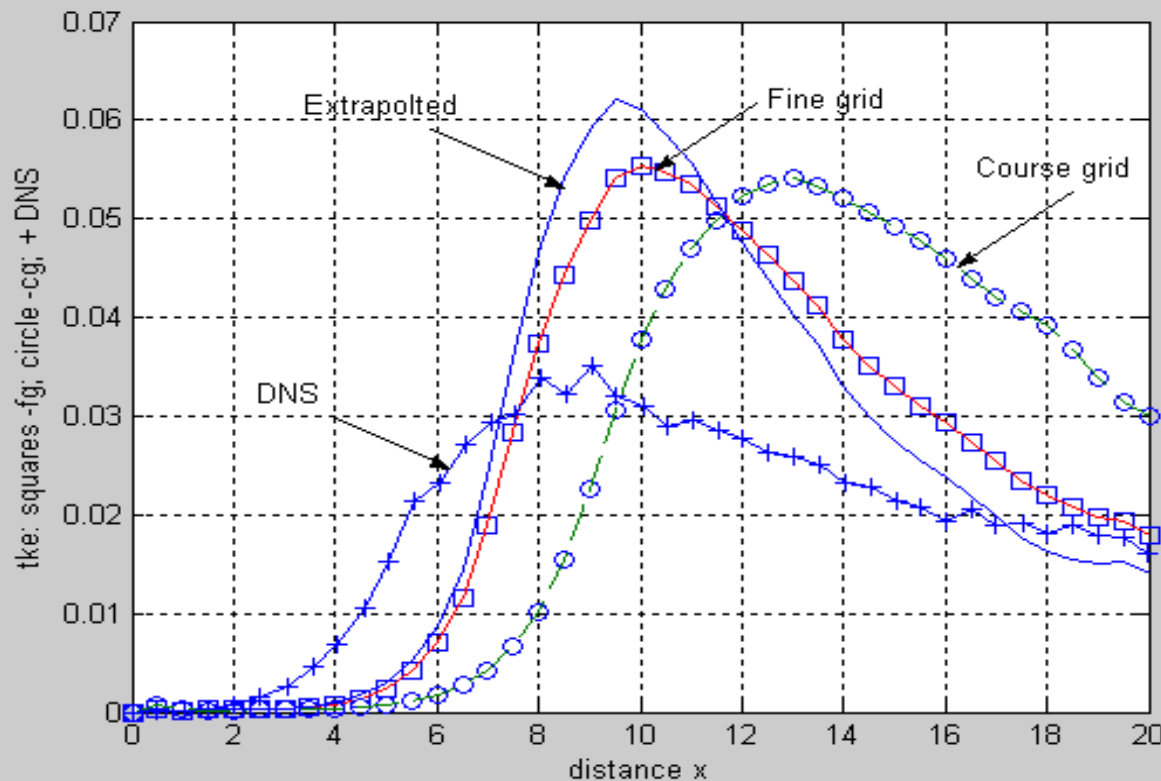
Transition in a Plane jet:



Turbulent kinetic energy profiles for a plane jet: DNS

Data: courtesy of Dr. Ing. Markus Klein (2005)

Transition in a Plane jet & Eff-Viscosity

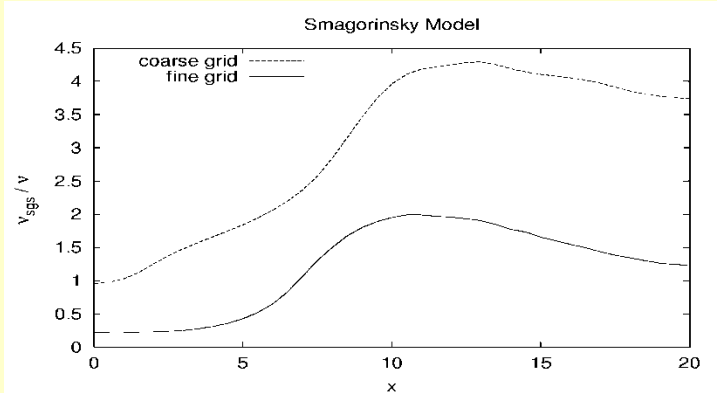


SSM

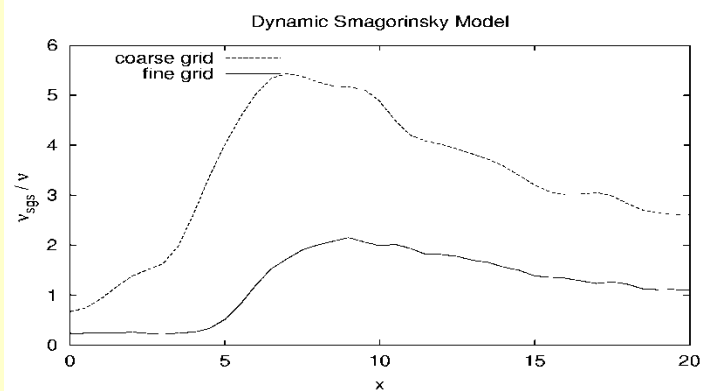
Comment: resolved tke should increase as grid is refined, or should it ?

Resolved turbulent kinetic energy profiles, (Klein et al, 2005); Smagorinsky model, $Re = 4000$ (based on inlet velocity = 1.0 m/s and nozzle diameter = 1.0m)

Importance of Numerical Viscosity

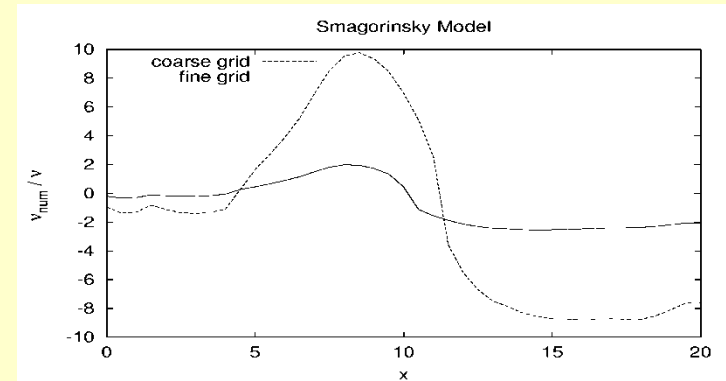


a

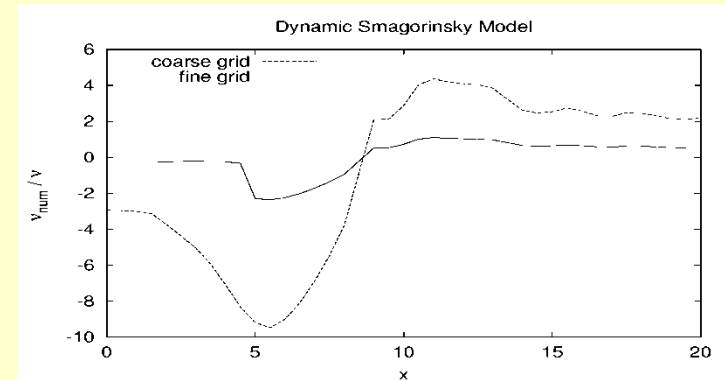


b

Sgs-viscosity obtained from plane jet LES data.



a



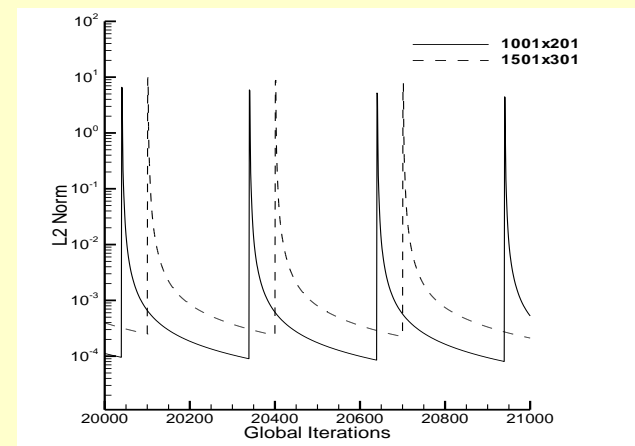
b

Estimated numerical viscosity normalized by laminar viscosity for plane jet LES data: (a) SSM, (b) DSM

Error Analysis: Iterative Convergence

Goal: Reduce normalized residual 3-4 orders of magnitude

- L2_norm of approximate iteration error > L2(Residuals)
- Eigenvalue of the solution matrix is important; Approximate iteration error is given by



Variation of L_2 -norm with iterations (after Huebsch, 2005)

$$\varepsilon_{iter}^n \cong \frac{|\phi^{n+1} - \phi^n|}{\lambda_1 - 1}$$

$$\lambda_1 \cong \frac{\|\phi^{n+1} - \phi^n\|}{\|\phi^n - \phi^{n-1}\|}$$

Error Analysis: Grid Convergence

Goal: Quantification of discretization errors

$$\phi_h = \phi_0 + \sum_{k=1}^{\infty} C_k x_h h^k \quad C_k x_h = \left(\frac{\partial \phi_h}{\partial h} \right)_{h=0}$$

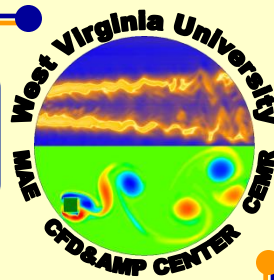
$$h = \Delta x \Delta y \Delta z \Delta t^* \quad h = \Delta x^2 + \Delta y^2 + \Delta z^2 + (\Delta t^*)^2$$

$$\phi_h = \phi_{ext} + ch^p \quad \phi_h = \phi_{ext} + c_1 h + c_2 h^2$$

$$\Delta t^* = u_{ch} \Delta t$$

(3 grid study is needed to determine p, c, and ϕ)

Error Analysis: Richardson Extrapolation-1

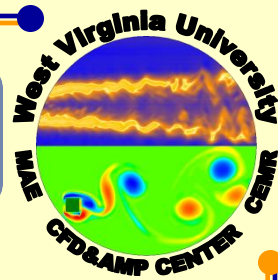


$$\phi = \phi_{ext} + ch^p \quad ; \text{ observed order } p \quad p = \frac{\ln \left\{ \frac{|\phi_3 - \phi_2|}{|\phi_2 - \phi_1|} \right\}}{\ln r}$$

Variants: Celik et. al. (2005), Eca and Hoekstra (2004), Orozco et al (2004), Celik and Karatekin (1997),
e.g.: Restrict $0 < p < 5$; but $p = -6$ means something (see next slide)

Perform at least 4-grid calculations and treat the outcome-as statistically random outcomes (Least squares, Eca et al, 2003-2004).

Richardson Extrapolation & Numerical Uncertainty: GCI Proposed by P. Roache



$$GCI = \frac{F_s}{r^p - 1} |f_2 - f_1|; \quad GCI\% = \frac{GCI}{|f_1|}$$

Table 1. Proposed implementation of the GCI for solutions on three or more systematically-refined grids using Equation (47).

$\left \frac{\hat{p} - p_f}{p_f} \right $	F_s	p
≤ 0.1	1.25	p_f
> 0.1	3.0	$\min(\max(0.1, \hat{p}), p_f)$

Using a global order works better!

Uncertainty estimation methods

- Grid Convergence Index (GCI)

$$U_{\phi}^f = 1.25 \left| \frac{\phi_{ext} - \phi_f}{\phi_f} \right|$$

- Coefficient of variation

For least squares

$$\sigma_r = \sum_{i=1}^n [\phi_i - (\phi_{ext} + \alpha h_i^p)]$$

standard error of the fit

$$\sigma_{\phi/h} = \sqrt{\sigma_r / (n-3)}$$

$$CV = \left| \frac{\sigma_{\phi/h}}{\phi_{ext}} \right|$$

For the other methods using triplets

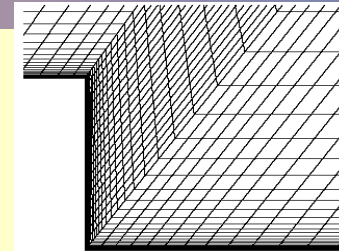
$$\mu = \sum_{i=1}^n \phi_{ext,i} / n$$

$$\sigma = \sqrt{\sum_{i=1}^n (\phi_{ext,i} - \mu)^2 / (n-1)}$$

$$CV = \left| \frac{\sigma}{\mu} \right|$$

$$ERE_{CV} = ERE + CV$$

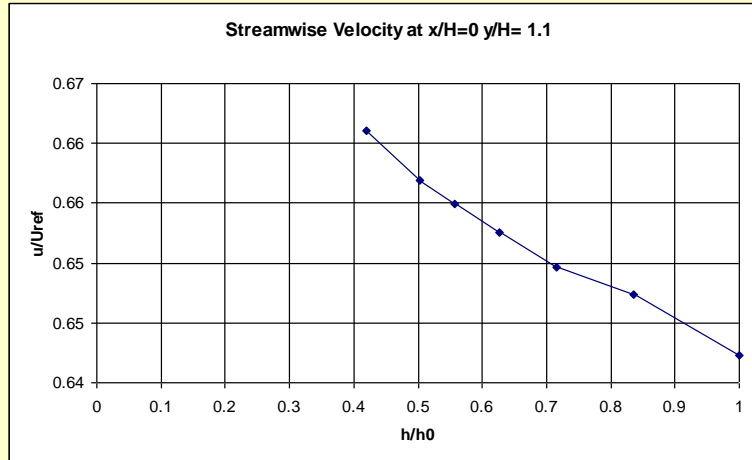
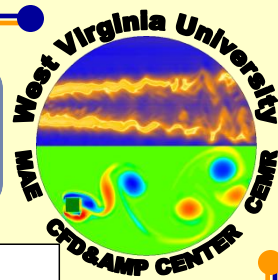
Example: Backward Step Flow



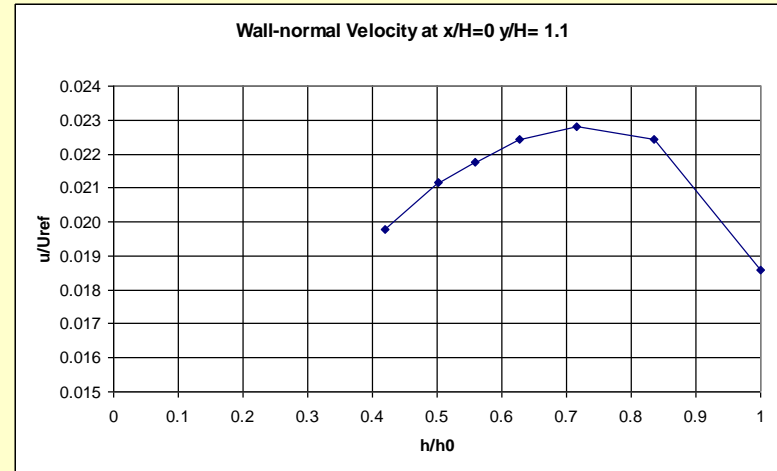
grids	ratio		grids	Ratio		Grids	Ratio		grids	ratio
101*101			101*101			141*141			101*101	
121*121	1.20		141*141	1.40		181*181	1.29		141*141	1.40
141*141	1.17		201*201	1.43		241*241	1.33		181*181	1.29
161*161	1.14								241*241	1.33
181*181	1.13									
201*201	1.11									
241*241	1.20									

- The four sets of grids used to calculate the extrapolation with least square method are 101-141-181-241

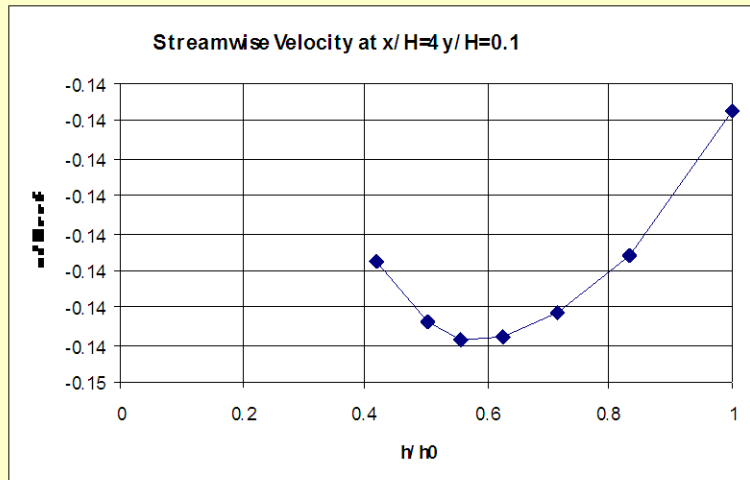
Convergence patterns --monotonic and oscillatory



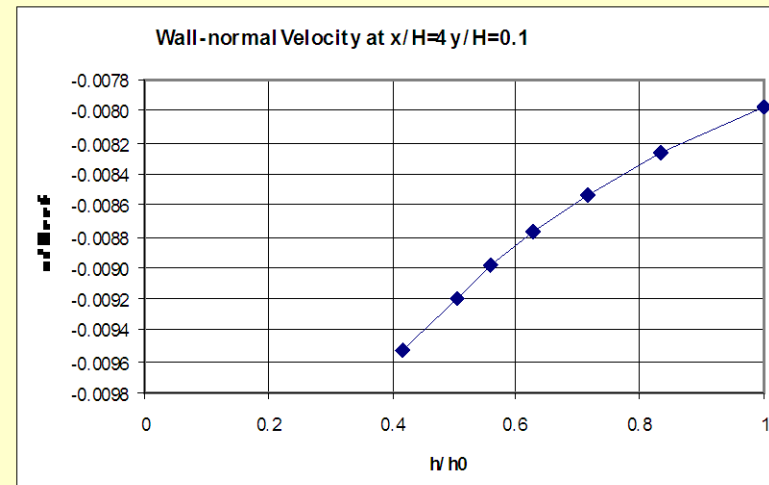
Streamwise vel. at (0,1.1)



Wall-normal vel. at (0,1.1)



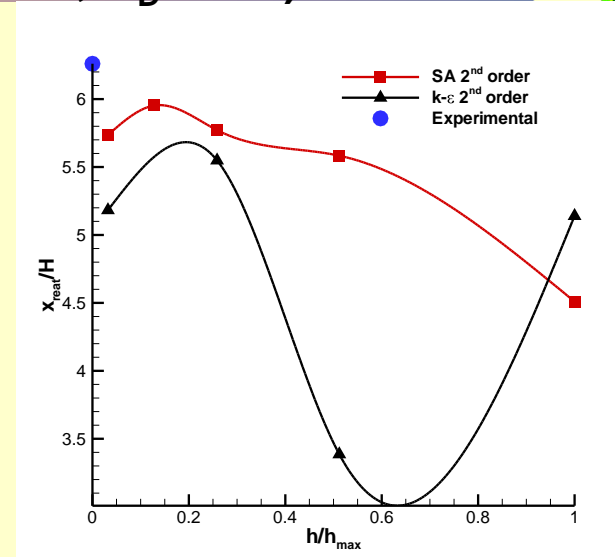
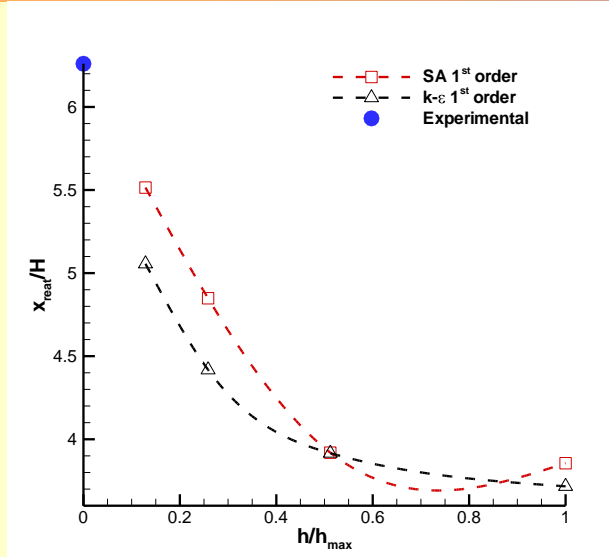
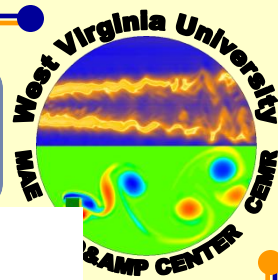
Streamwise vel. at (4,0.1)



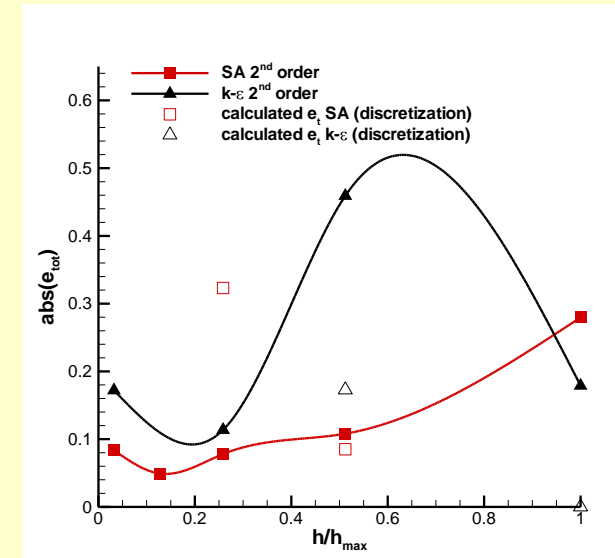
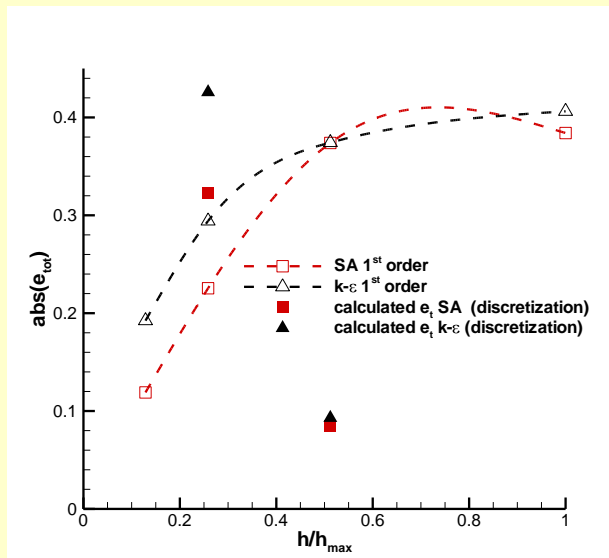
Wall-normal vel. at (4,0.1)

Flow Over a Backward Facing Step

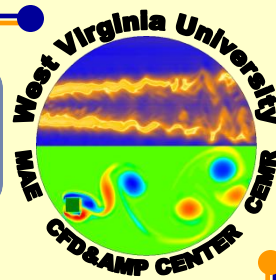
Reattachment Point ($D=6.26$, $U_D=10\%$)



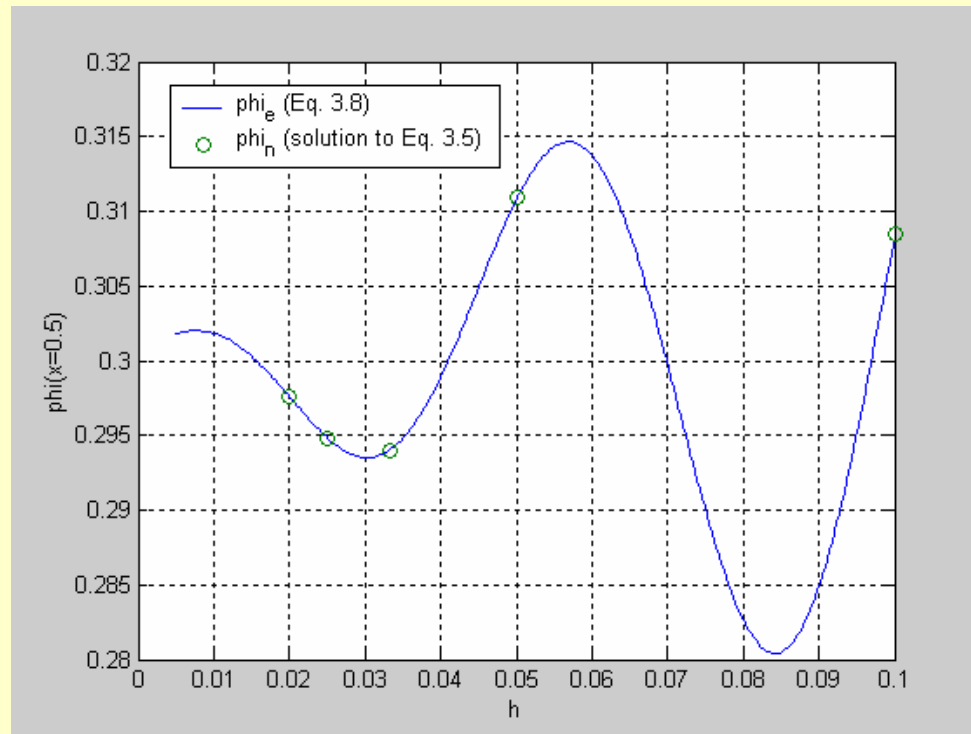
Total Error in Estimation of Reattachment Point



Oscillatory Convergence: Manufactured FDE (Celik etal, 2005)



$$u\phi_x = \phi_{xx} - \lambda\phi \quad \text{with } \phi(0) = 0 \quad \phi(1) = 1$$



$$-a_i\tilde{\phi}_{i-1} + b_i\tilde{\phi}_i - c_i\tilde{\phi}_{i+1} = 0$$

$$b_i = a_i + c_i + \lambda \quad (1)$$

$$\text{Assume } a_i = c_i + \frac{u_i}{h} \quad (2)$$

$$E_i \equiv \tilde{\phi}_i - \phi_i = g_i f$$

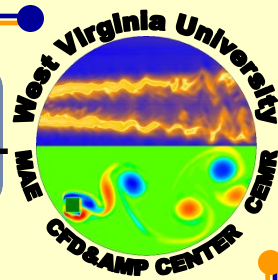
$$f = h^p \cos(kh)$$

$$g_i = \beta(i-1)(nx-i)$$

$$-a_i(\phi_{i-1} + g_{i-1}f) + b_i(\phi_i + g_i f) - c_i(\phi_{i+1} + g_{i+1}f) = 0 \quad (3)$$

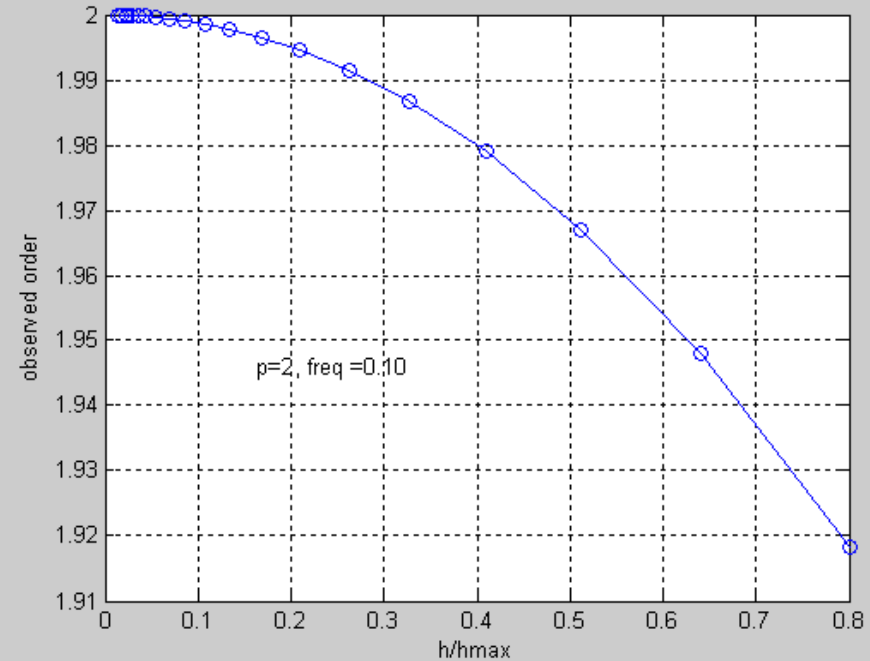
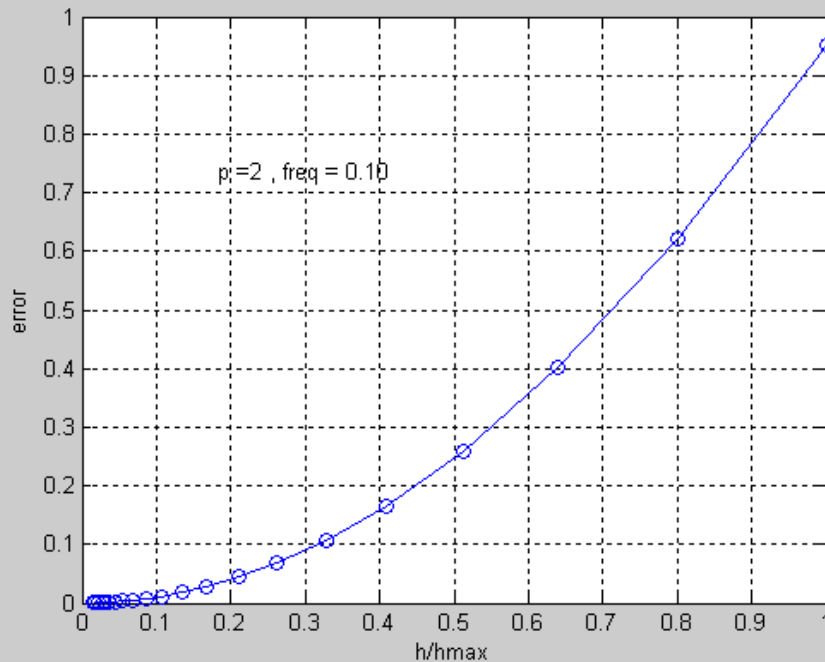
a_i , b_i and c_i can be solved by combining (1-3)

Error Analysis: Richardson Extrapolation-4

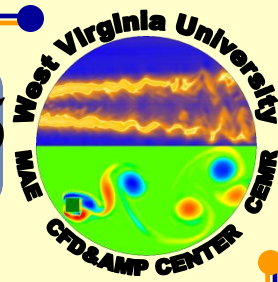


Oscillatory convergence examples

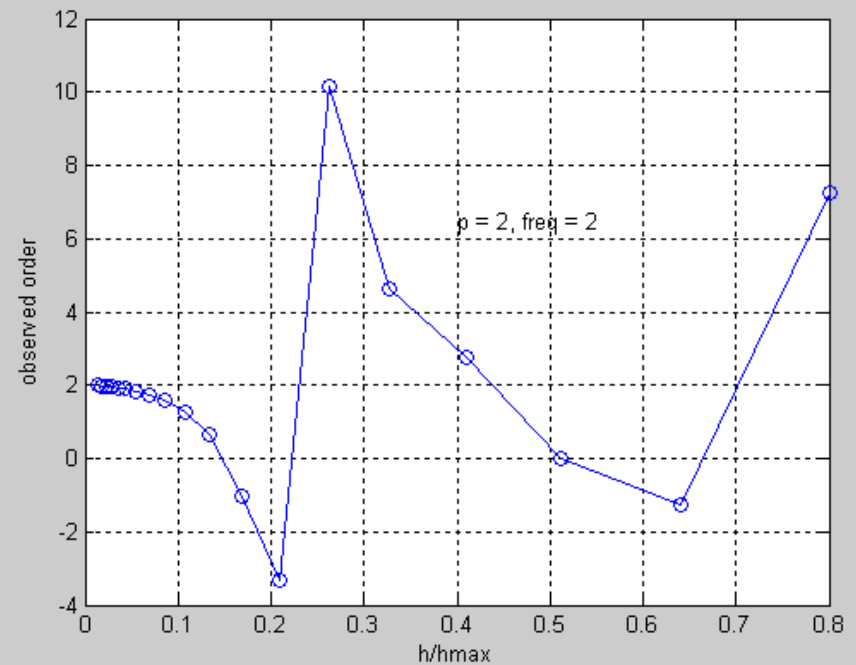
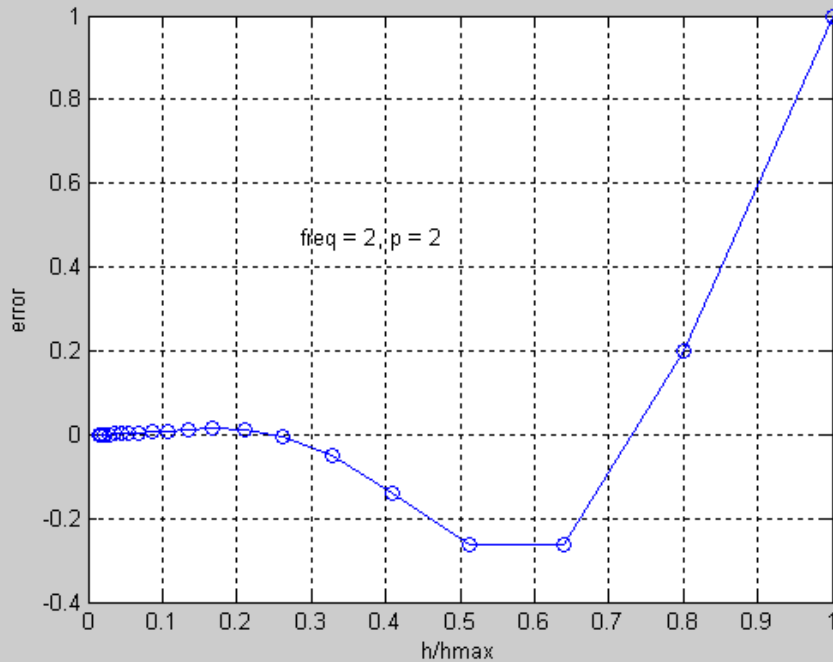
$$\phi_h = \phi_0 + gh^p \cos 2\pi fh$$



Error Analysis: Richardson Extrapolation-5



Oscillatory convergence examples



AES: An Alternative Error estimation method (Celik et al, 2008)

Present method assumes that the true error E_t is proportional to the approximate error, E_a

$$E_t^h = cE_a^h$$

For a three grid (triplet) calculation:

True error: $E_t^h = \phi - \phi_h$

$$\alpha_1 = h_2/h_1$$

$$\alpha_2 = h_3/h_2$$

Approximate error: $E_a^h = \phi_h - \phi_{ch}$

$$h_1 < h_2 < h_3$$

Local proportionality constants:

$$c_{i,j}^1 = \frac{\phi_2^{i,j} - \phi_1^{i,j}}{\phi_3^{i,j} - 2\phi_2^{i,j} + \phi_1^{i,j}} \quad \text{Fine-medium meshes}$$

$$c_{i,j}^2 = \frac{\phi_3^{i,j} - \phi_2^{i,j}}{\phi_3^{i,j} - 2\phi_2^{i,j} + \phi_1^{i,j}} \quad \text{Medium-coarse meshes}$$

Global proportionality constant:

$$c = \frac{1}{2} \frac{\|c_{i,j}^1\|_\infty + \|c_{i,j}^2\|_\infty}{N}$$

$$\|c_{i,j}\|_\infty = \sum_{k=1}^N |c_{i,j}|$$

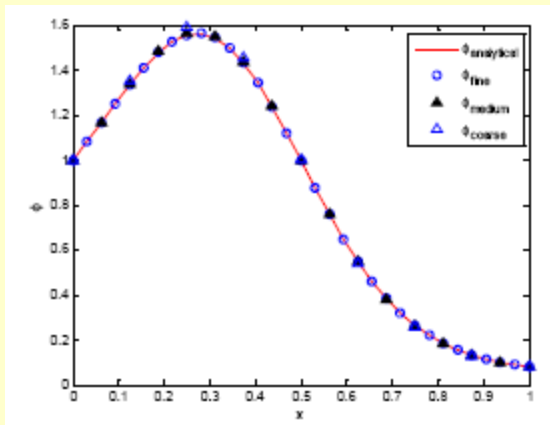
N : # of grid points

Example Application of the AES(Approximate Error Scaling Method

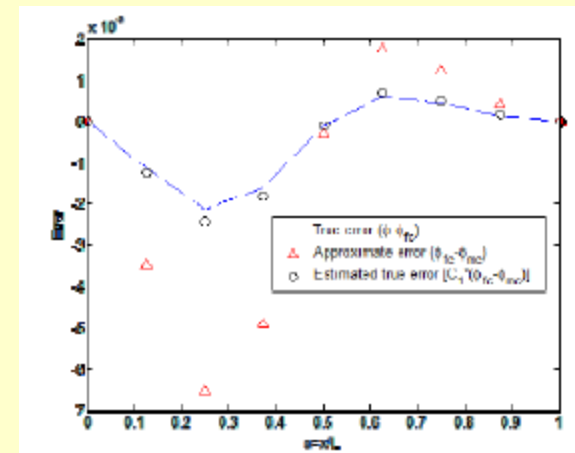
$$\frac{d}{dx}(u\phi) = \frac{d}{dx}\left(\Gamma \frac{d\phi}{dx}\right) + S_\phi$$

$$u = \bar{u} \cos(\omega x)$$

$$\phi = \exp\left(\frac{ux}{\Gamma}\right)$$

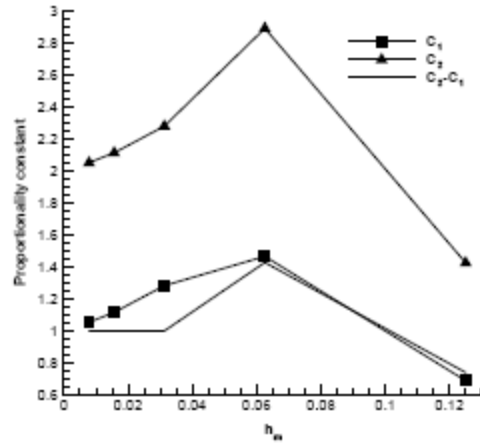


Analytical and numerical solutions of the scalar

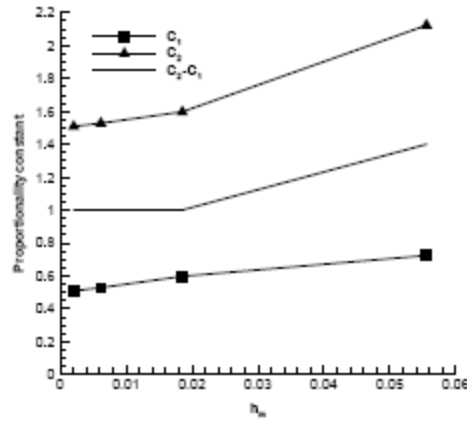


True error, approximate error and estimated true error

Approach to Asymptotic Range

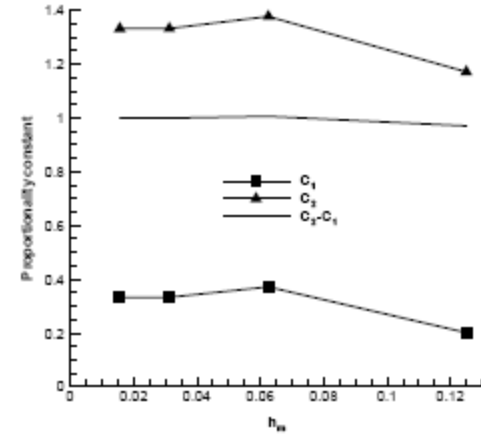


(a)

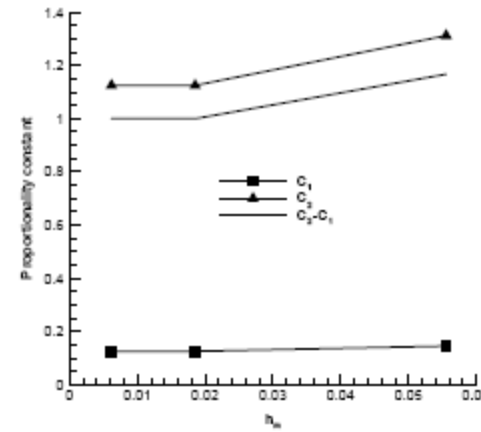


(b)

Upwind scheme for convective terms with refinement factors of (a) 2 and (b) 3



(a)



(b)

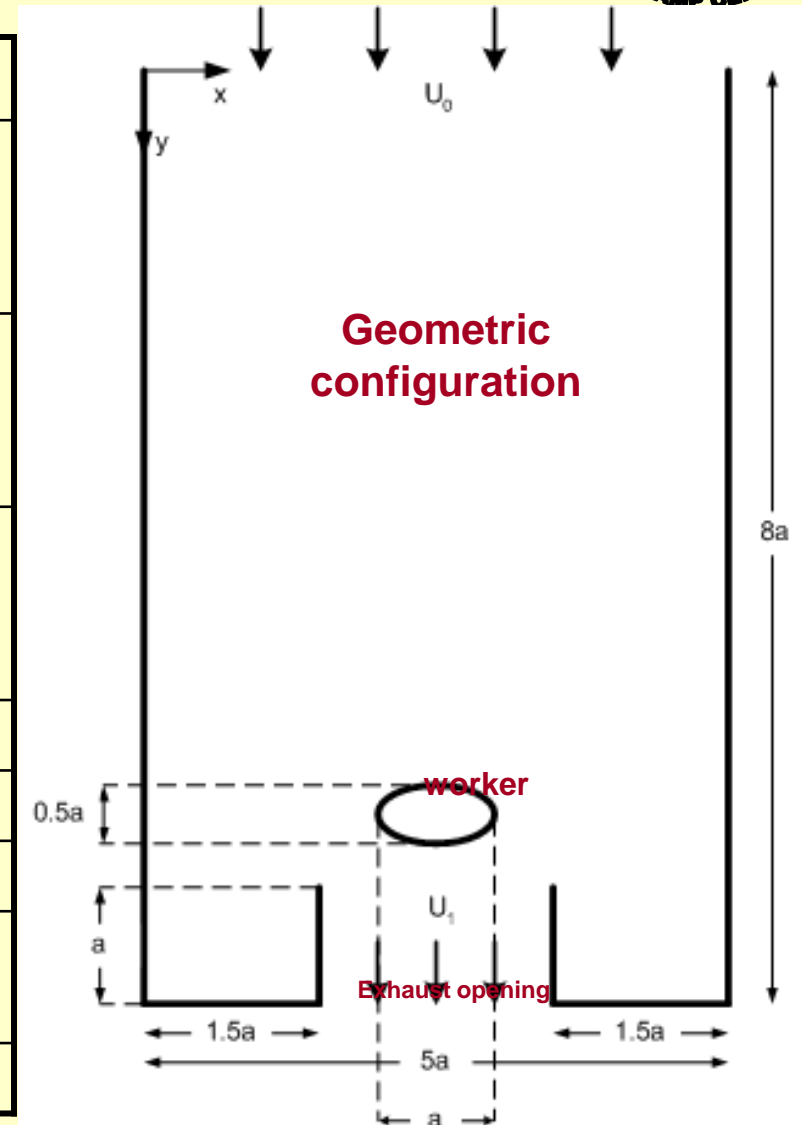
Central differencing for convective terms with refinement factors of (a) 2 and (b) 3

2D flow around an ellipse (with contraction in the downstream)

Proposed by Dunnett (1994)

Simulation Details

Reynolds number	100,000 10,000 1,000
$Re = aU_0/2\nu_{air}$	
Turbulence models	Standard k- ϵ RNG k- ϵ SST k- ω
Inlet velocity (U_0)	5m/s 0.5m/s 0.005,/s
Time step	0.006 s
Total time	40 s
Vel.-Pres. Coupling	SIMPLEC
Scheme	QUICK for conv. 2 nd order cent for diff
Residuals	1×10^{-4}



2D flow around an ellipse (with contraction in the downstream)

Grid dependency of parameters relevant to flow separation

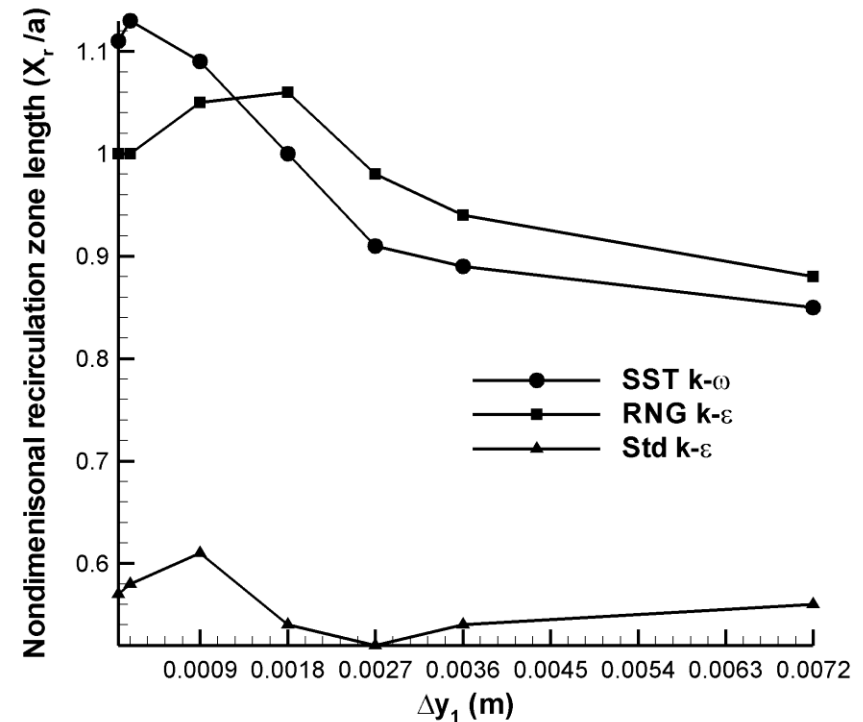
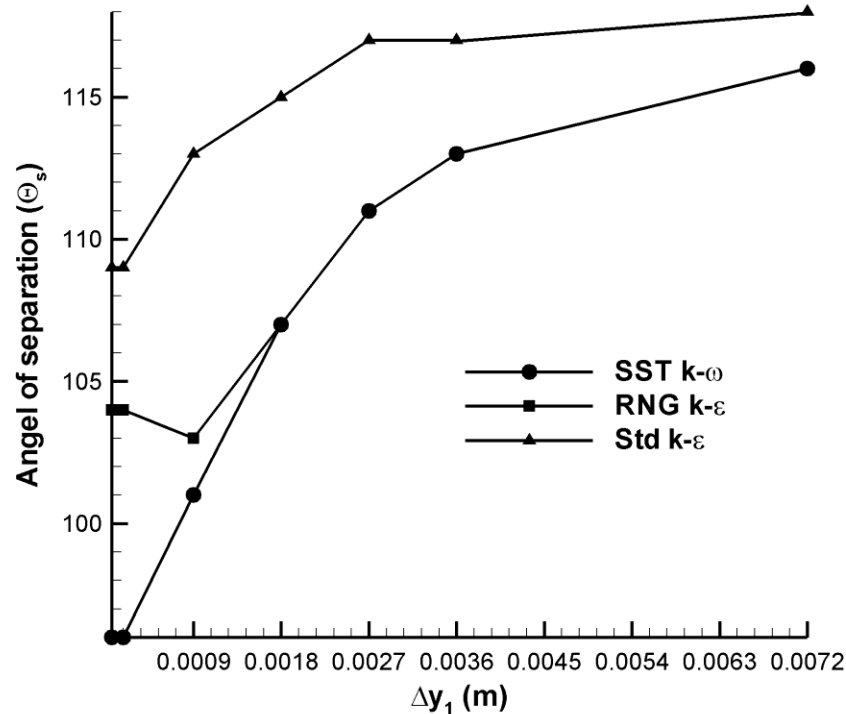
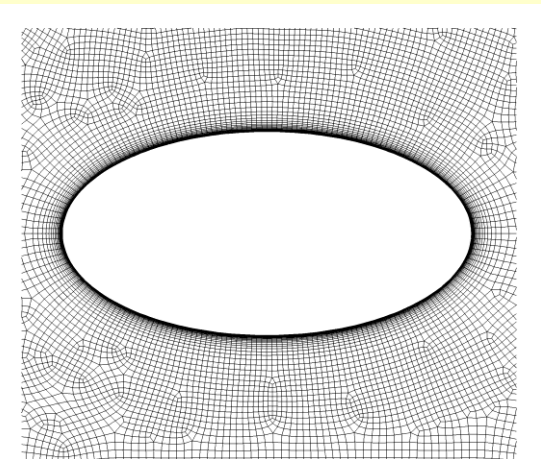


Table: Number of cells used in two-dimensional simulations

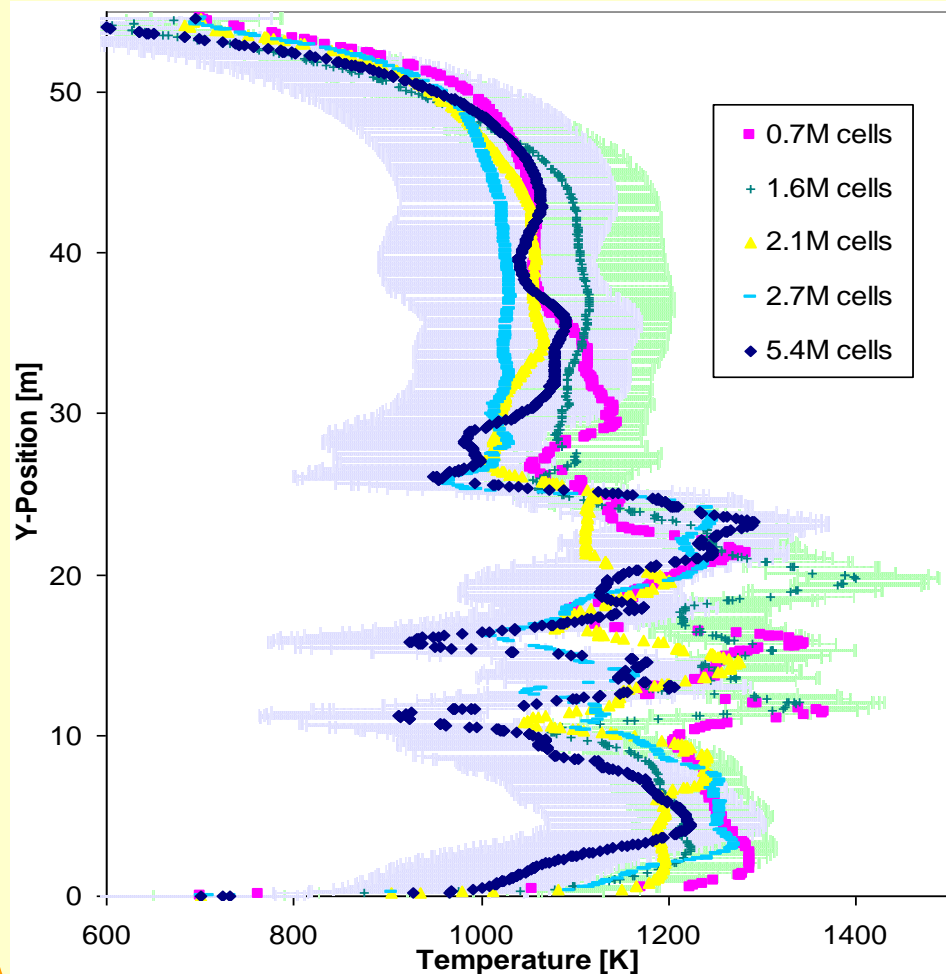
Grid	$Re = 1.0 \times 10^5$	$Re = 1.0 \times 10^4$	$Re = 1.0 \times 10^3$
G1	9,594 ($\Delta y_I = 7.2 \times 10^{-3} \text{m}$)	51,144 ² ($\Delta y_I = 4.6 \times 10^{-4} \text{m}$)	51,144 ² ($\Delta y_I = 4.6 \times 10^{-4} \text{m}$)
G2	24,993 ($\Delta y_I = 3.6 \times 10^{-3} \text{m}$)		
G3	49,037 ($\Delta y_I = 2.7 \times 10^{-3} \text{m}$)		
G4	59,340 ¹ ($\Delta y_I = 1.8 \times 10^{-3} \text{m}$)		
G5	76,663 ¹ ($\Delta y_I = 9.0 \times 10^{-4} \text{m}$)		
G6	81,081 ¹ ($\Delta y_I = 1.8 \times 10^{-4} \text{m}$)		
G7	93,883 ¹ ($\Delta y_I = 6.0 \times 10^{-5} \text{m}$)		

¹: Enhanced wall treatment used in $k-\varepsilon$ model calculations

²: Transitional flow modifications are enabled in SST $k-\omega$ model calculations

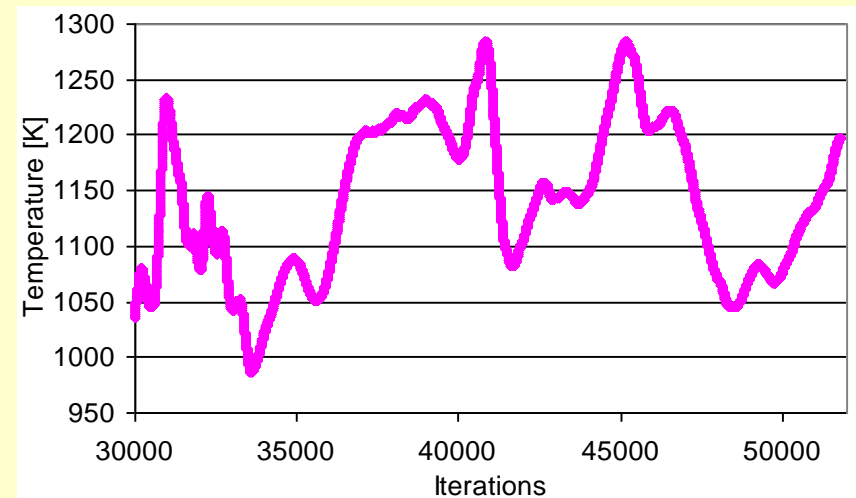


650MW Boiler Simulations



Dashed blue and green lines show the temperature error bars for the 5.4M and 1.6M cells, respectively

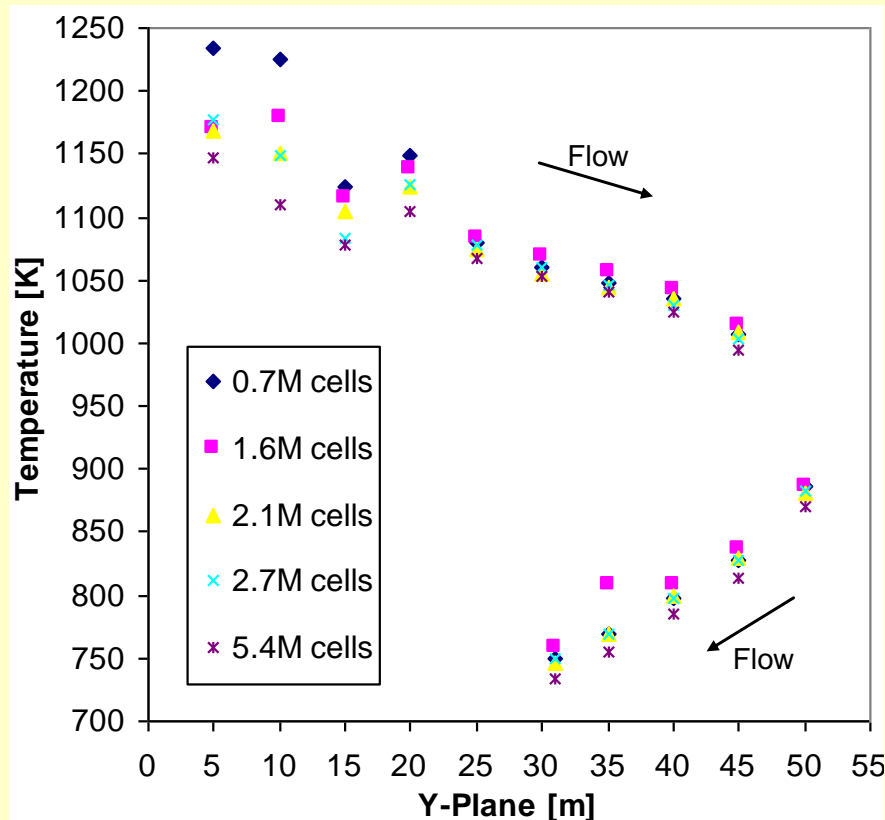
Error bars obtained from temperature monitor at central point in burners zone



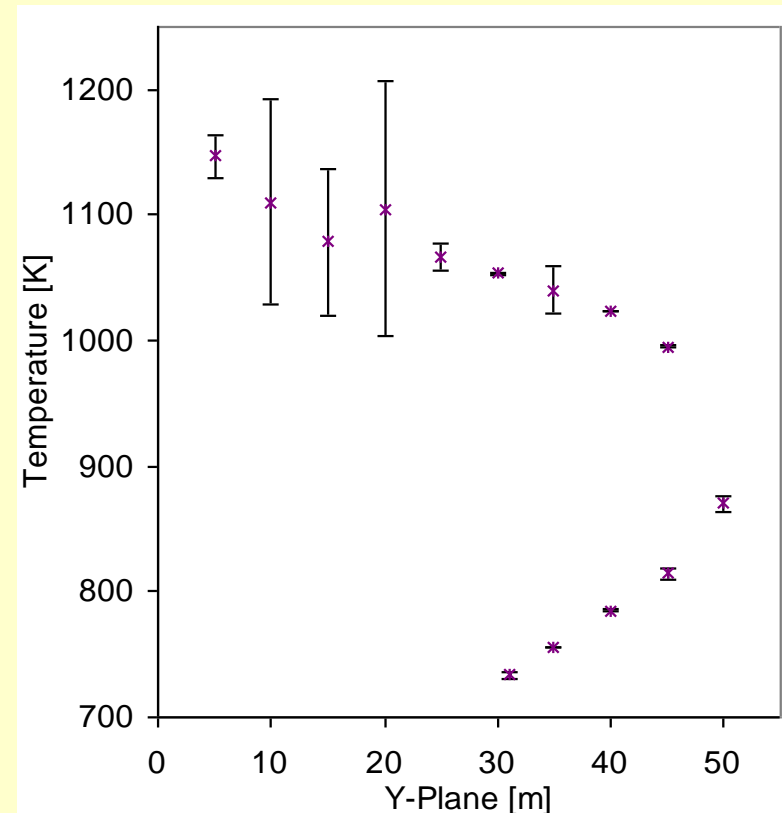
Temperature along the symmetrical line

Temperature monitor at a burner point in the 5.4M cells-grid

Discretization Uncertainty

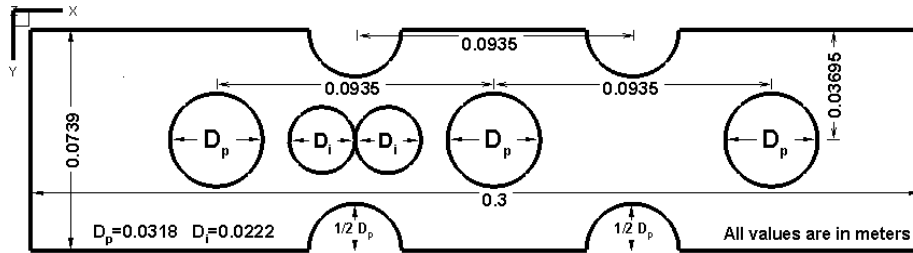


Bulk-Mean Temperatures at Horizontal Cross Planes

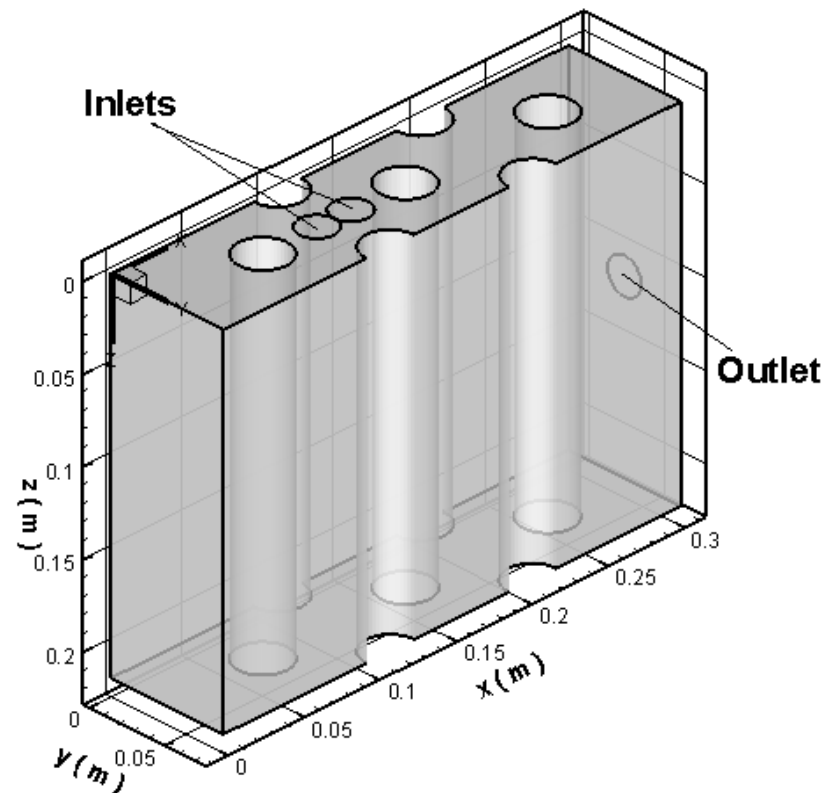


Local apparent order 0.6-14.6,
 $p_{ave}=5.46$
 Maximum discretization
 uncertainty 9.3% ($\pm 102K$)

Sketch of the flow plenum (top view)



3-Dimensional perspective



3D structured boundary layers, extending 20% of the pole diameter, D_p

Average $y^+ < 5$

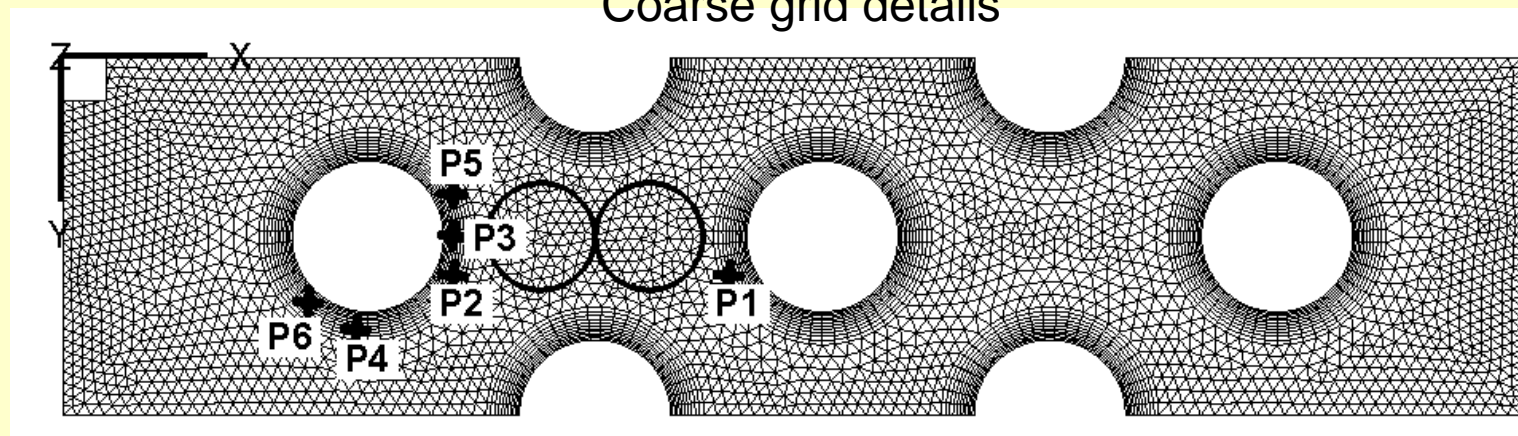
Enhanced wall treatment in the near wall region

Rest of the domain : unstructured tet-mesh

Mesh coarsening factor, r , of ~ 1.5

593,928 (coarse), 873,493 (medium), and 1,186,944 (fine) cells

Coarse grid details



Flow Details

	Low-Re	High-Re
Inlet velocity of a single jet	1.611×10^{-1} m/s	5.660×10^{-1} m/s
Total flow rate	1.246×10^{-4} m ³ /s	4.382×10^{-4} m ³ /s
Average plenum velocity	7.739×10^{-3} m/s	2.720×10^{-2} m/s
Flow through time (FTT)	32s	9s
Total execution time	450s (~14 FTT)	250s (~28 FTT)
Pole Reynolds number	245	431

Turbulence models

: RNG k- ϵ , SST k- ω

Residuals

: 1×10^{-4}

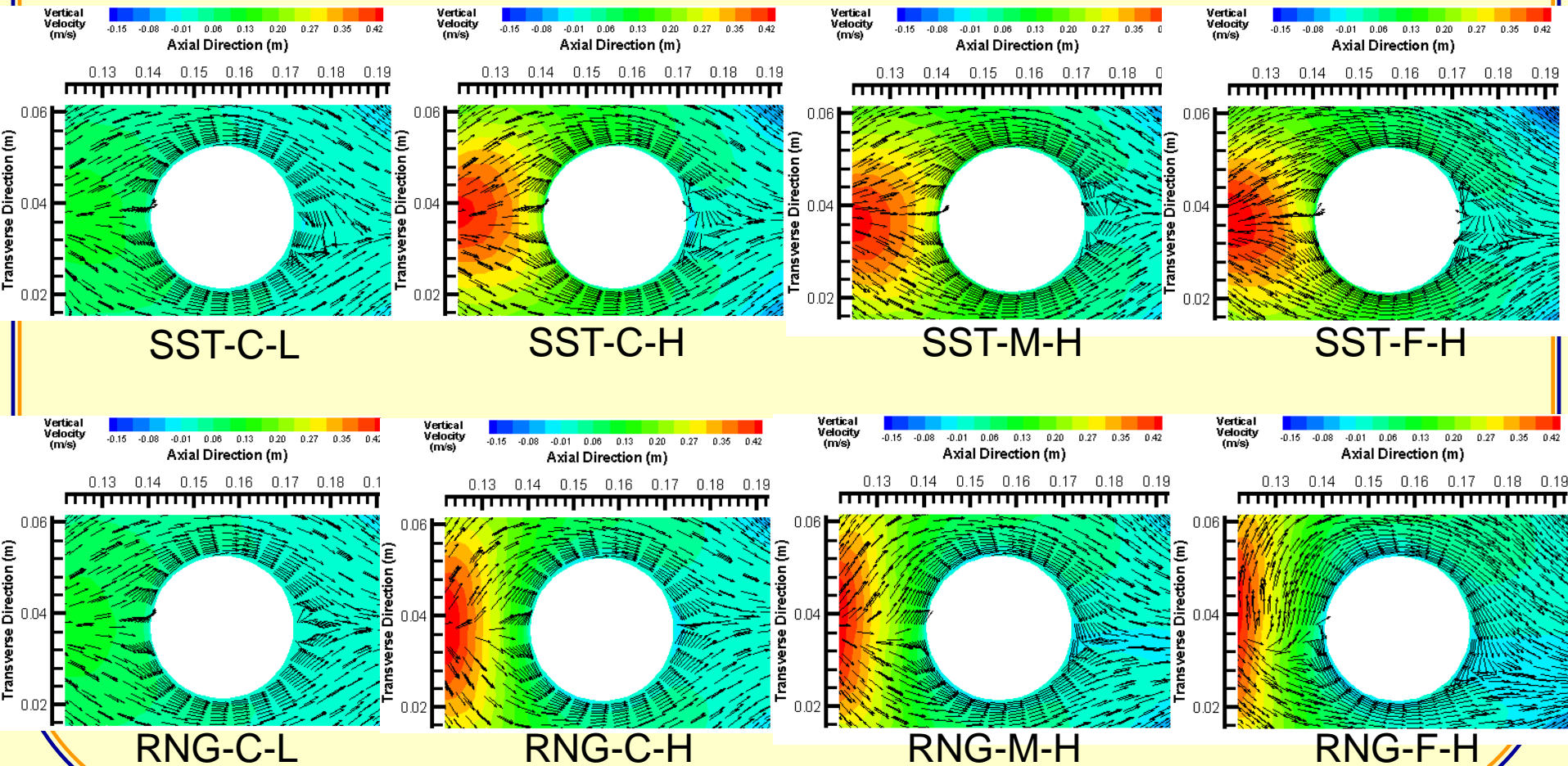
Time step

: 1×10^{-3} s

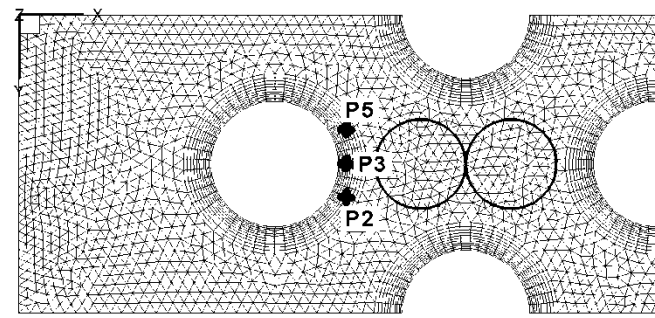
Numerical Schemes

: 2nd order upwind (Conv.), 2nd order central (Diff.)
2nd order (Pressure) , 1st order (time)

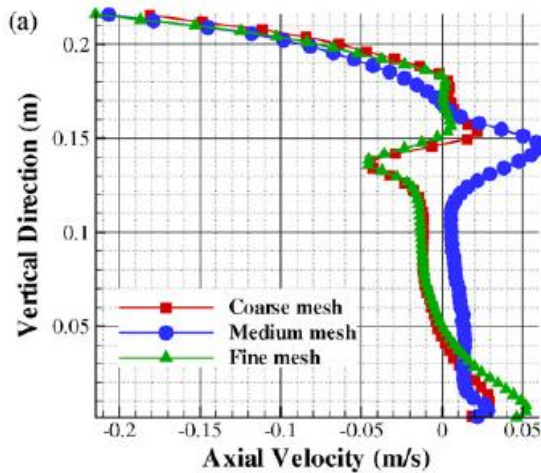
Separation from middle rod



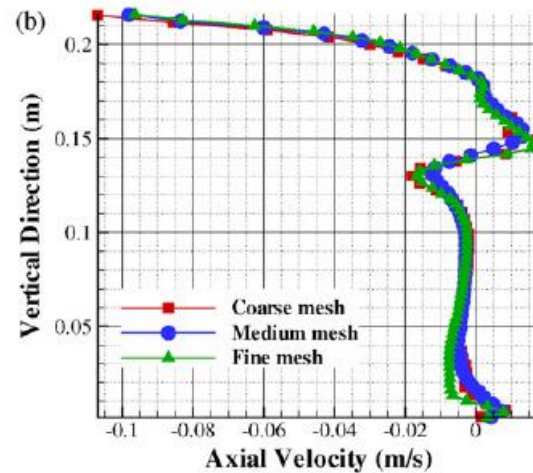
Ensemble ave. of axial velocity profiles over the last 100s
SST $k-\omega$ (top row), and RNG $k-\varepsilon$ (bottom row)



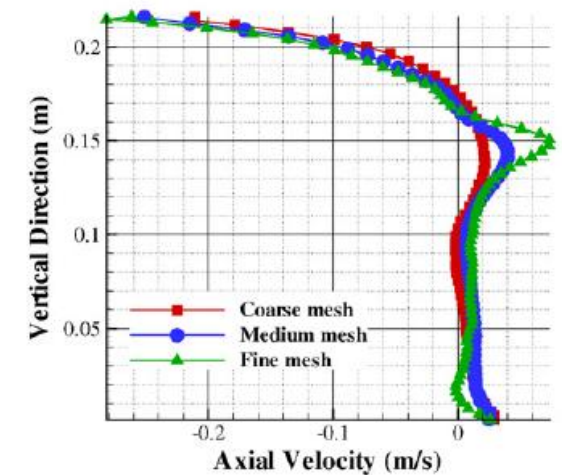
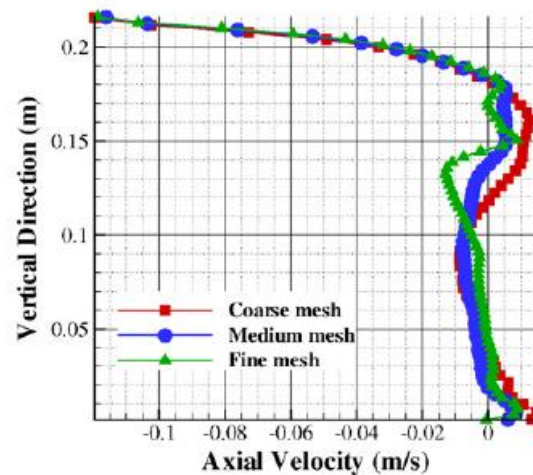
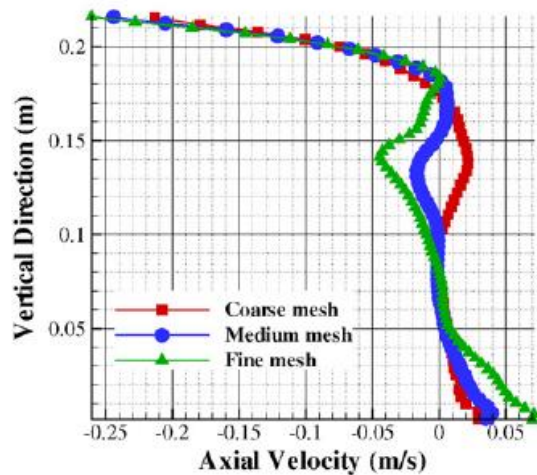
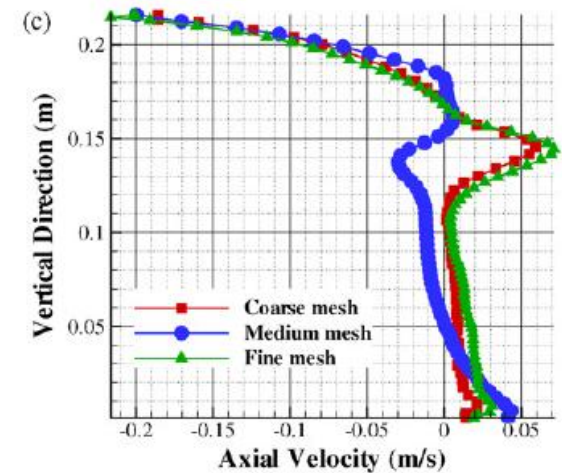
P2



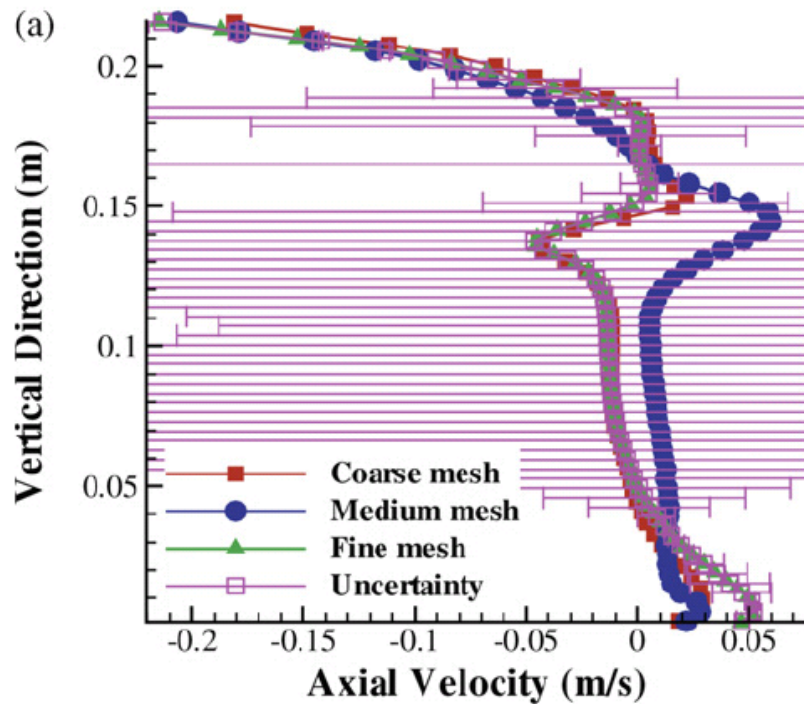
P3



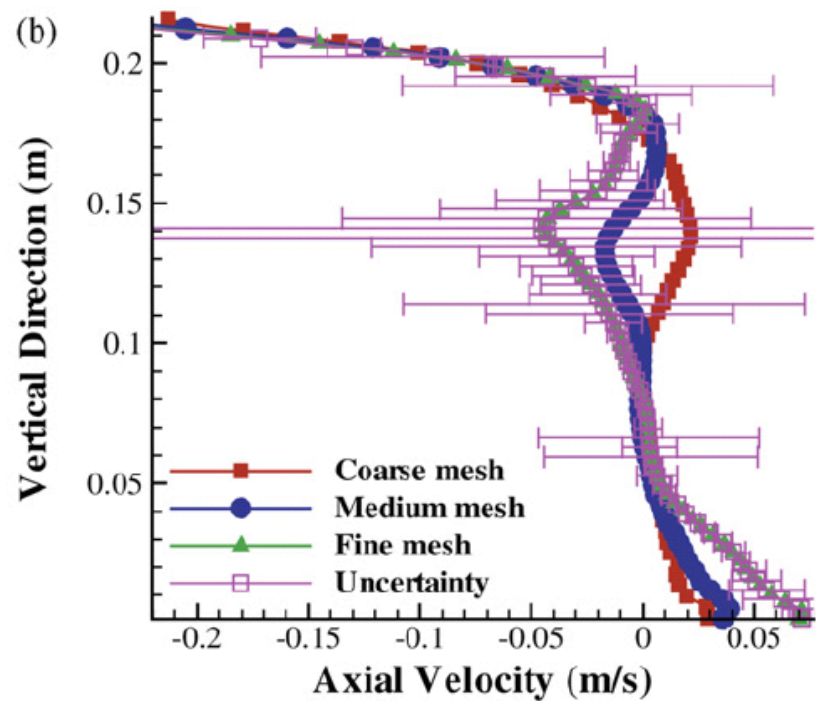
P5



Predicted uncertainties with JFE method at P2

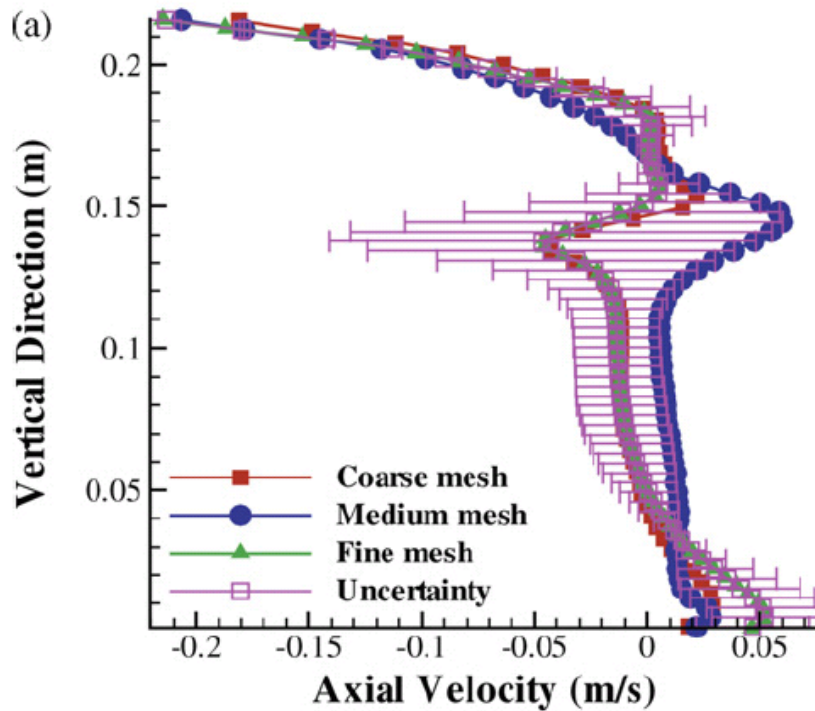


SST $k-\omega$ model

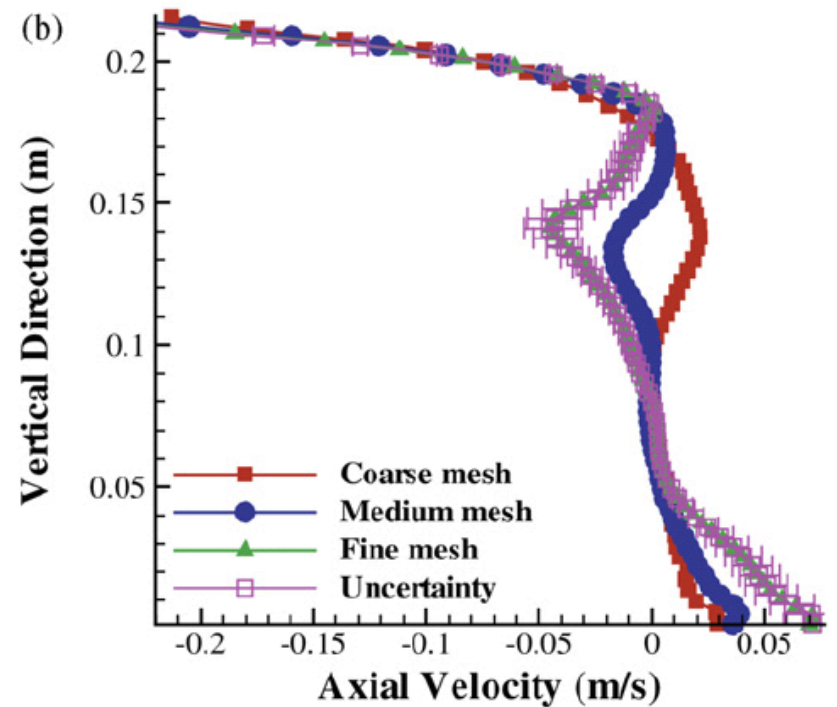


RNG $k-\varepsilon$ model

Predicted uncertainties with JFE method and averaged p (order) at P2

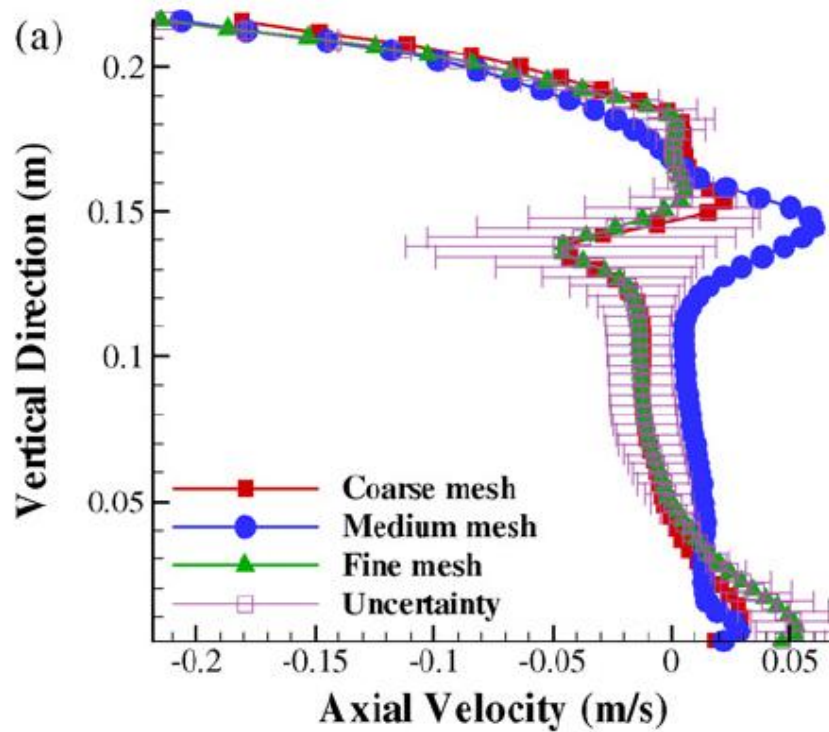


SST $k-\omega$ model

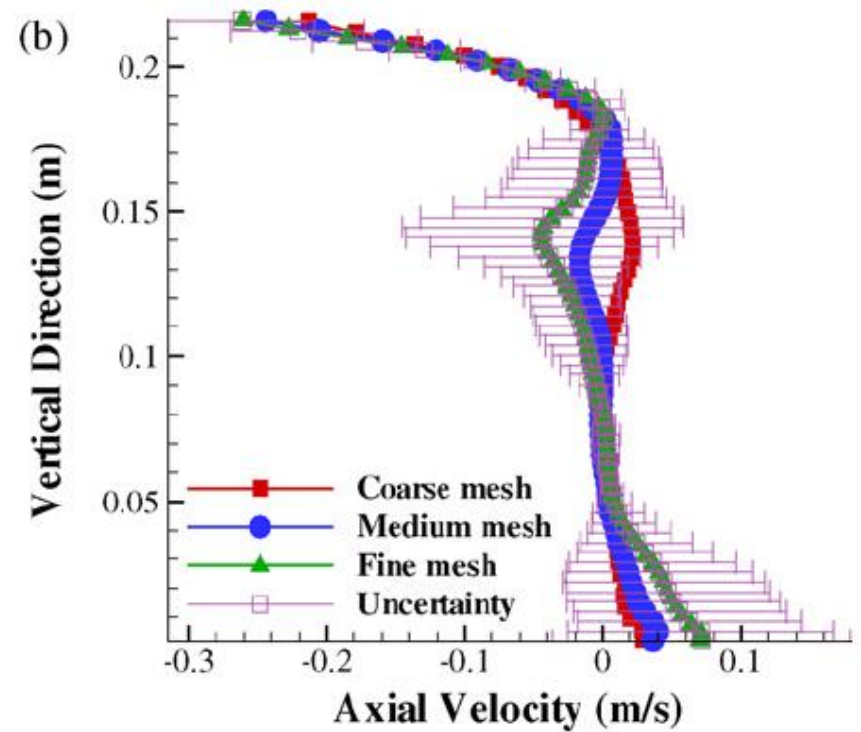


RNG $k-\epsilon$ model

Predicted uncertainties with AES method at P2

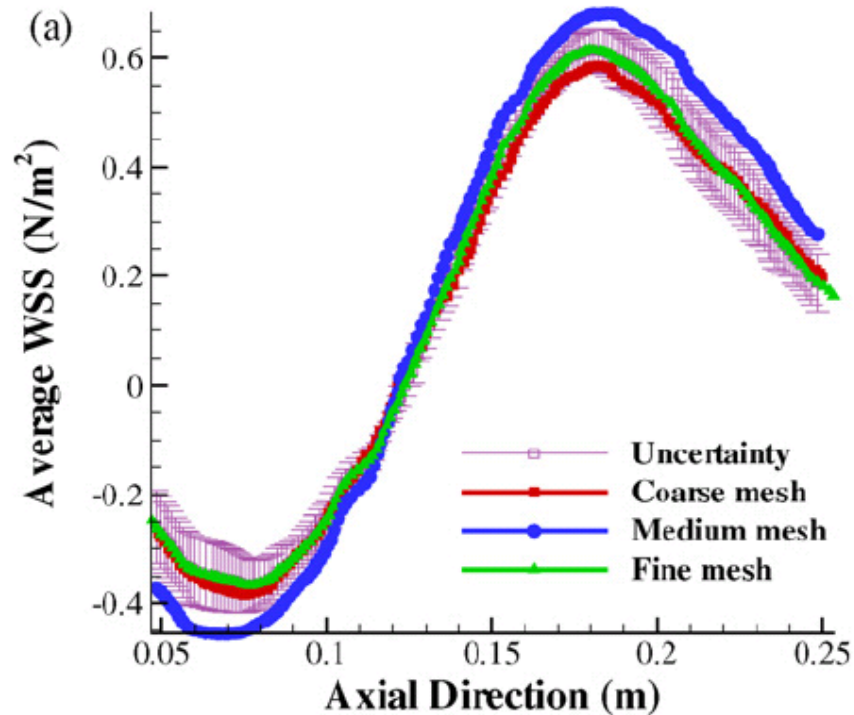


SST $k-\omega$ model

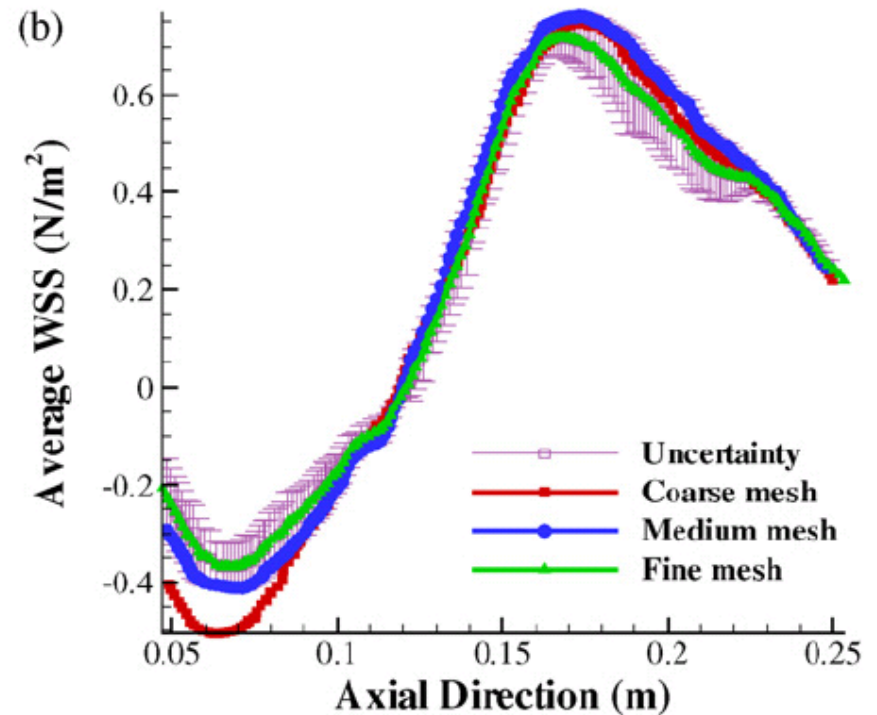


RNG $k-\epsilon$ model

Spatially filtered wall shear stress profiles and uncertainties by AES method at $y = 0.018475\text{m}$ $z = 0.2175\text{ m}$

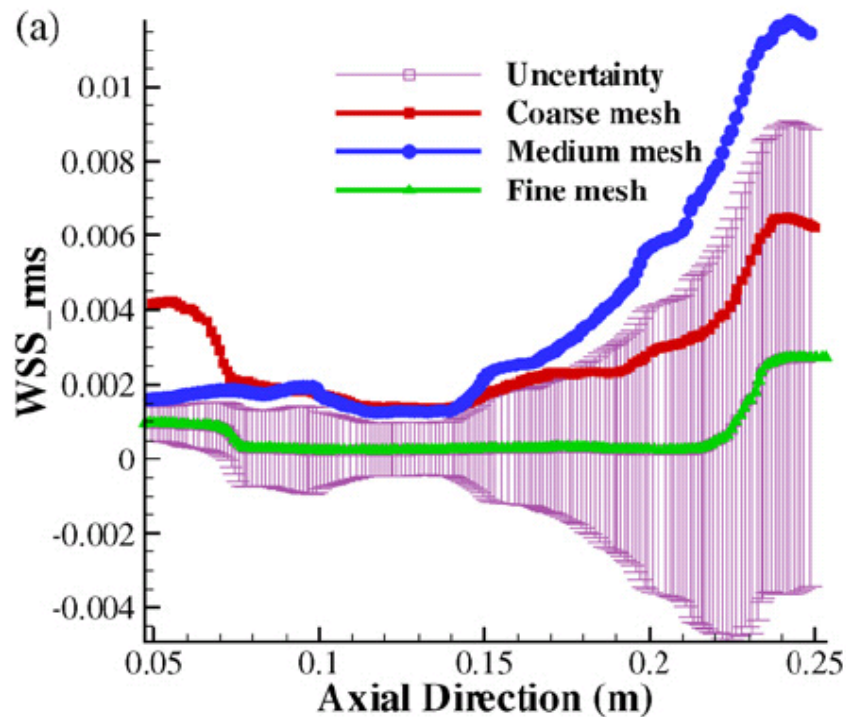


SST $k-\omega$ model

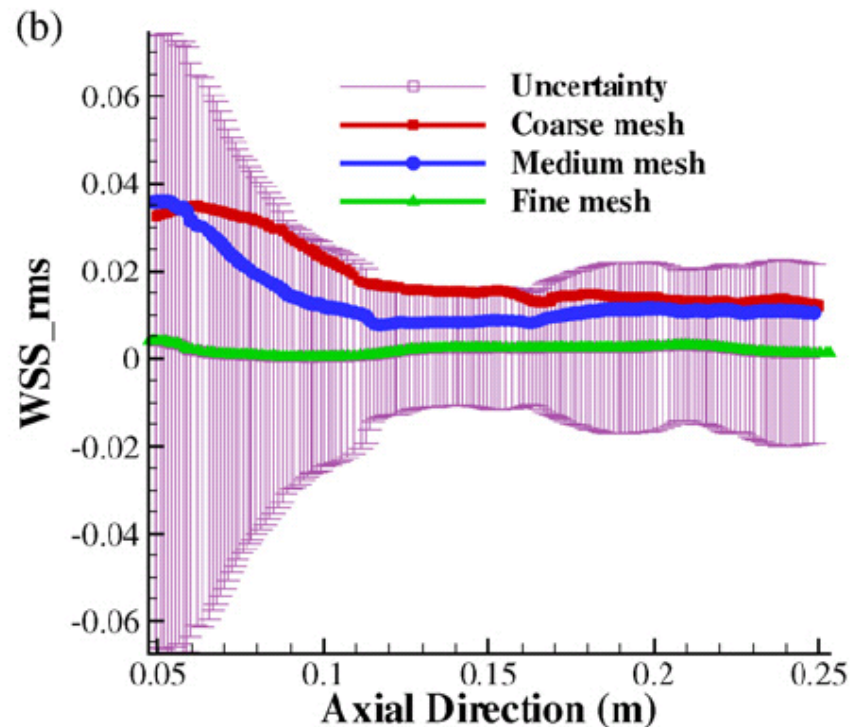


RNG $k-\varepsilon$ model

Spatially filtered *rms* wall shear stress profiles calculated using ensemble averaging along with the uncertainties by AES method at $y = 0.018475\text{m}$ $z = 0.2175\text{m}$



SST $k-\omega$ model



RNG $k-\varepsilon$ model

ETE vs. RE

Ref: Celik & Hu, 2004

- **Richardson extrapolation (RE)**
 - Popular, relatively reliable (+)
 - At least three sets of grid, expensive (-)
 - Difficult to identify asymptotic range (-)
 - Does not work for oscillatory grid convergence (-)
- **Error transport method (ETE)**
 - No extra effort in grid generation (+)
 - Can be solved using the same scheme (+)
 - Can be used as a post-processing tool for steady problems(+)
 - Additional recourses for code development (-)
 - Difficulty in determining source term of ETE (-)
 - Reliability still under investigation (-)

Literature review of ETE

- Roache (1993 & 1998)
- Van Straalen et al. (1995)
- Zhang et al. (1997)
- Wilson & Stern (2001)
- Celik & Hu (2002, 2003)
- Qin & Shih (2003)

Error Transport Equation (ETE)

Non-linear: $L(\phi) = 0$

Linearized: $L_h(\tilde{\phi}) = 0 \quad (1)$

$$L_h(\phi) = R = \tau(\phi) \quad (2)$$

L : differential operator (PDE)

L_h : difference operator (FDE)

ϕ : exact solution to PDE

ϕ^{\sim} : numerical solution

R : residual

error is defined as: $\varepsilon = \phi - \tilde{\phi}$

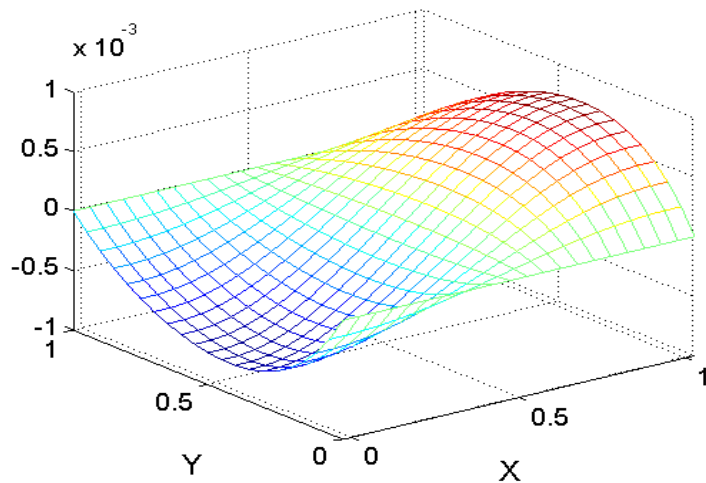
ETE: $L_h(\varepsilon) \equiv L_h(\phi) - L_h(\tilde{\phi}) = \tau(\phi)$

τ represents the truncation error of a discretized equation,
i.e. the *error source term*

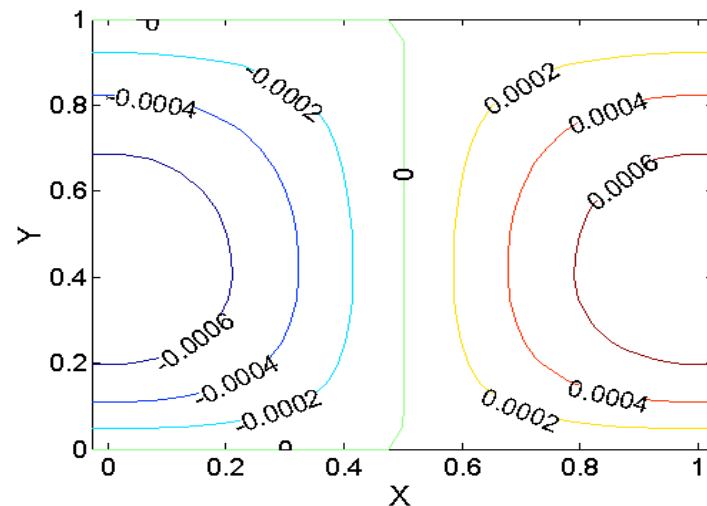
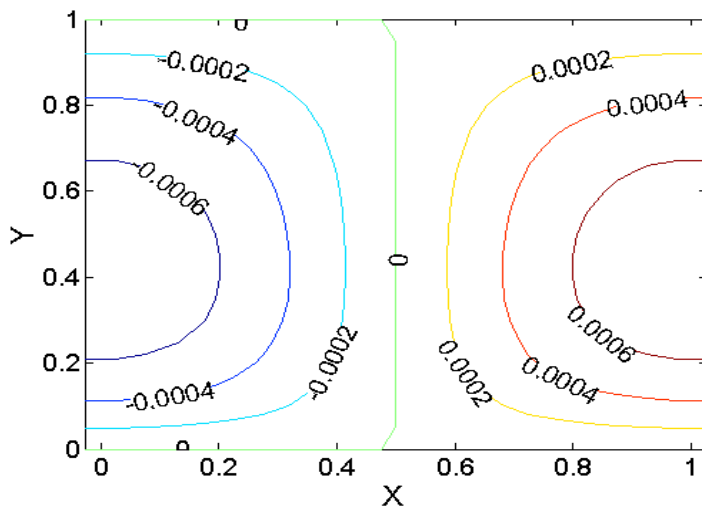
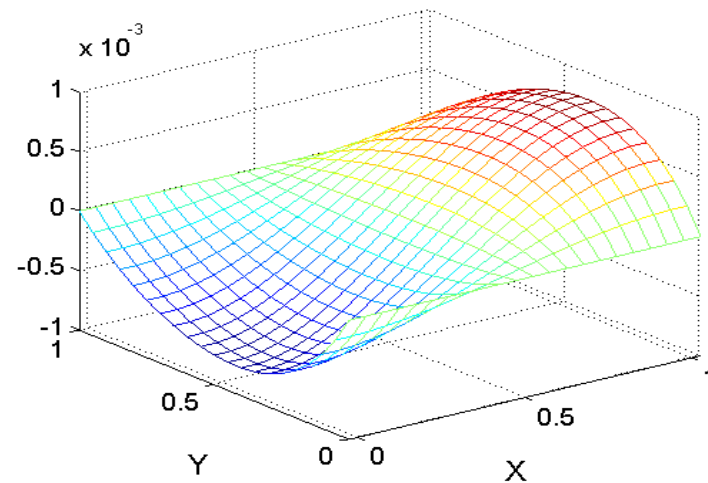
2D Poisson Equation:

Central difference Scheme

Exact error

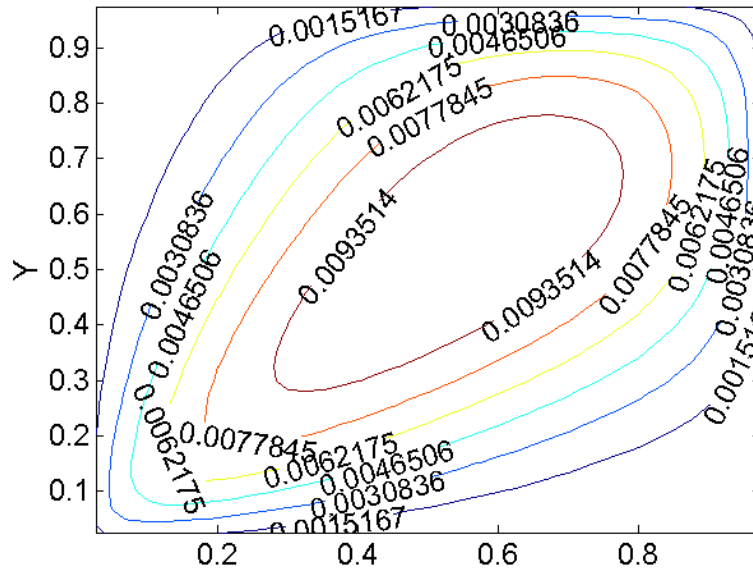
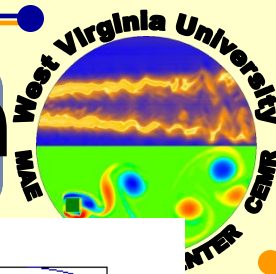


ETE error

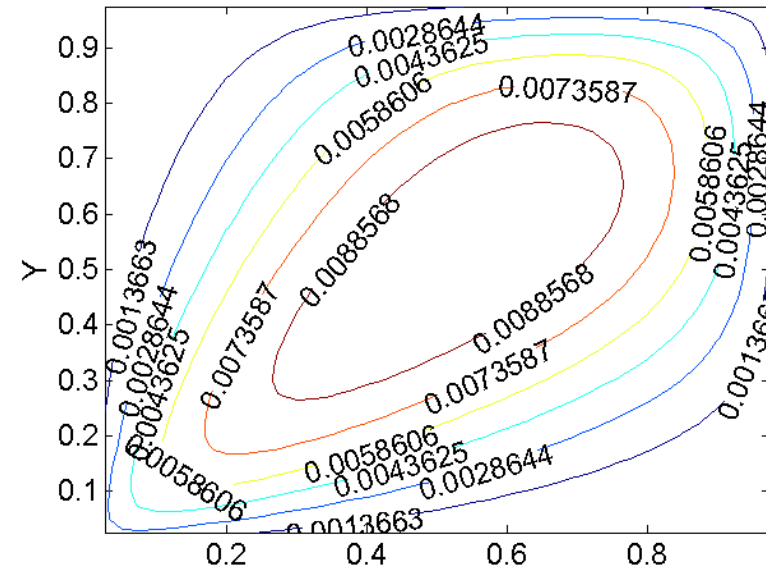


2D Steady Convection Diffusion

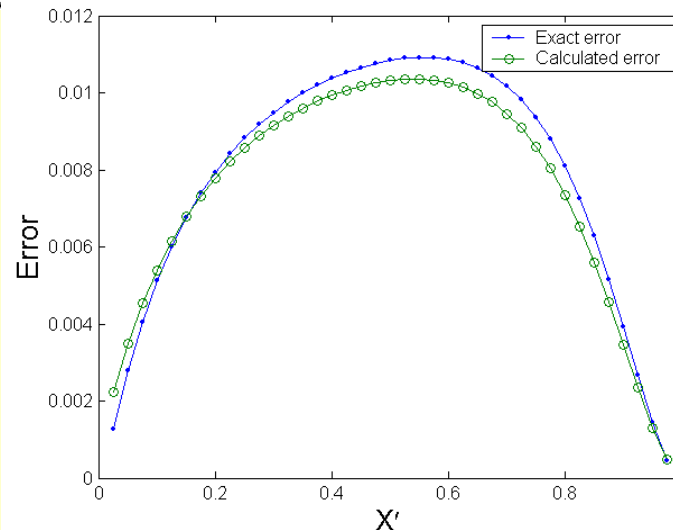
1st order Upwind scheme



Exact error

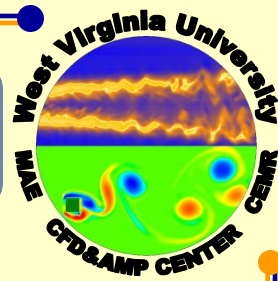


Calculated error



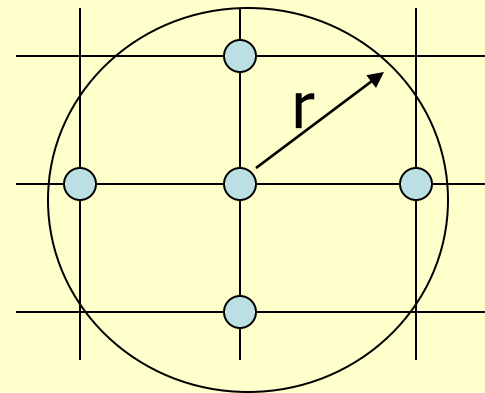
Line plot along diagonal

Generalized Derivation of Error Source



$$\left(\begin{array}{c} \text{implicit} \\ \text{coefficient} \\ \text{matrix} \end{array} \right) \left(\begin{array}{c} \phi^{\text{new}} \end{array} \right) = \left(\begin{array}{c} \text{explicit} \\ \text{coefficient} \\ \text{matrix} \end{array} \right) \left(\begin{array}{c} \phi^{\text{old}} \end{array} \right)$$

Influence circle \rightarrow



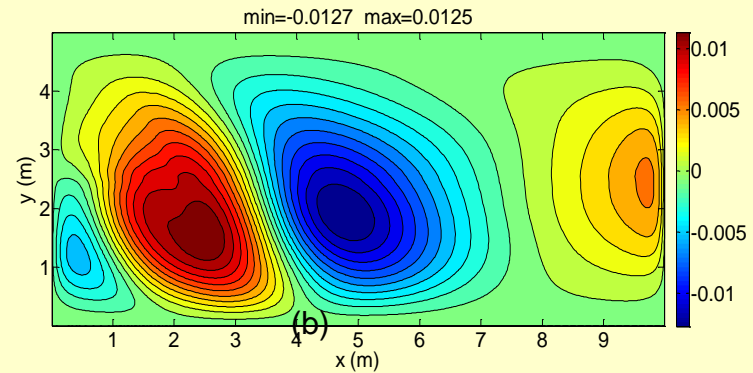
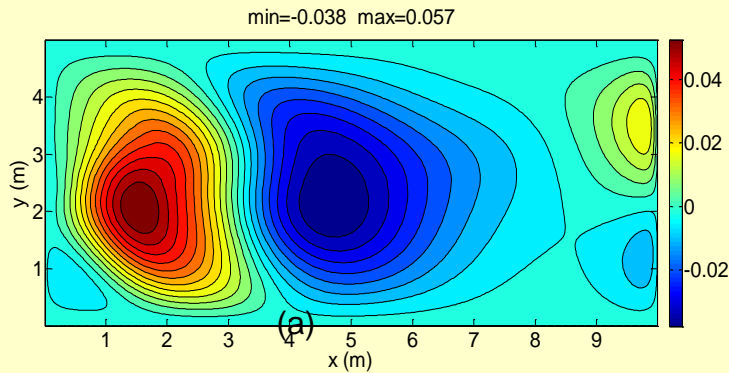
Need to know:

1. Access to the coefficient matrix
2. Influence circle (or radius)

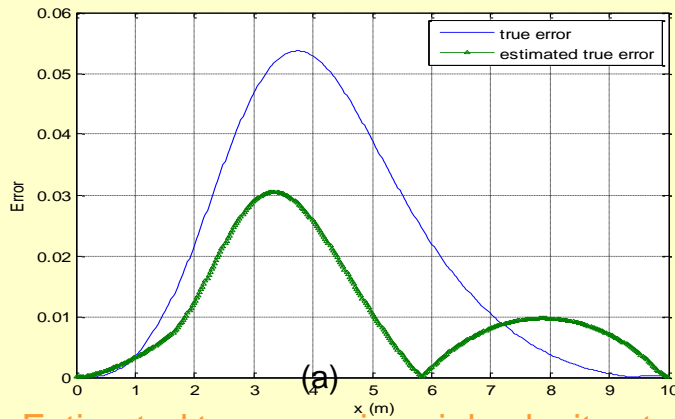
Conclusions

- For RANS, methods based on Richardson extrapolation are preferred for their robustness, however they do not always work and it is not easy to detect where and when they will fail.
- Although there is evidence that time step can be simply treated as another discretization parameter, it is much safer to use a relatively small time step so as to minimize its effect compared to space discretization.
- To quantify discretization errors at least 3-4 grid calculations are needed (may be 4-5 sets for oscillatory convergence); It may be erroneous to assume monotonic convergence just by observing the behavior of three or four points.
- *A hybrid of extrapolation and ETE methods is the way to go!*

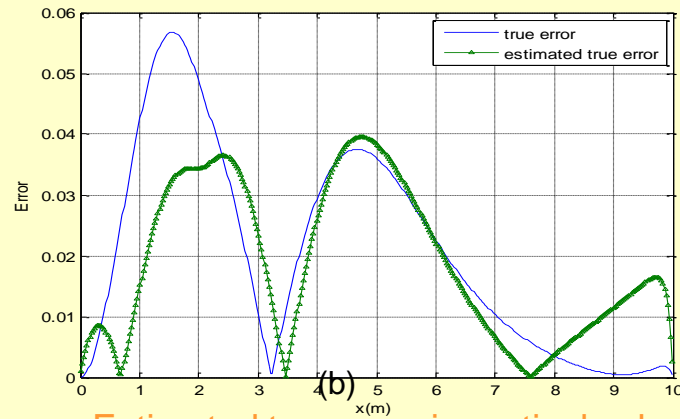
Example: Hybrid AES & ETE



Error in axial velocity (a) True error on medium grid, (b) Approximate error between fine and medium grid



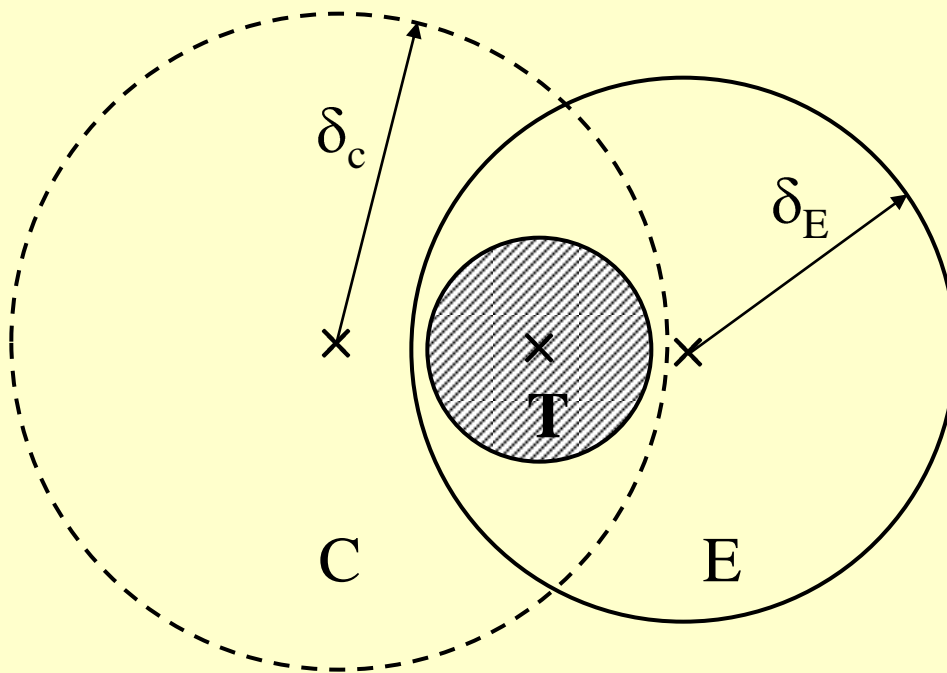
Estimated true error in axial velocity at (a) $x = 3.5\text{m}$, (b) $y = 1\text{m}$, (c) $y = 3.5\text{m}$



Estimated true error in vertical velocity at (a) $x = 1.5\text{m}$, (b) $x = 5\text{m}$, (c) $y = 2\text{m}$

Challenge

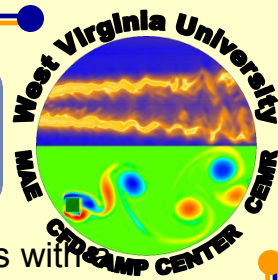
Predict the 'truth' within an acceptable confidence interval without knowing the 'truth'



“What can not be computed is meaningless!”

(Davies, 1992)

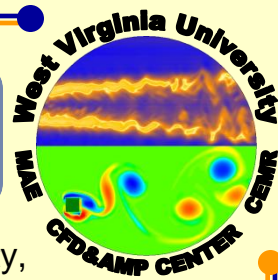
$T = \text{'truth'} \pm \text{fuzziness about truth}$



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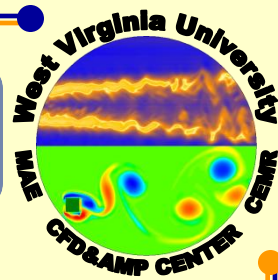
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